# LAMMPS Users Manual

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LAMMPS Documentation

Version info:

The LAMMPS "version" is the date when it was released, such as 1 May 2010. LAMMPS is updated continuously. Whenever we fix a bug or add a feature, we release it immediately, and post a notice on this page of the WWW site. Each dated copy of LAMMPS contains all the features and bug-fixes up to and including that version date. The version date is printed to the screen and logfile every time you run LAMMPS. It is also in the file src/version.h and in the LAMMPS directory name created when you unpack a tarball.

• If you browse the HTML doc pages on the LAMMPS WWW site, they always describe the most current version of LAMMPS.
• If you browse the HTML doc pages included in your tarball, they describe the version you have.
• The PDF file on the WWW site or in the tarball is updated about once per month. This is because it is large, and we don't want it to be part of every patch.
• There is also a Developer.pdf file in the doc directory, which describes the internal structure and algorithms of LAMMPS.

LAMMPS stands for Large-scale Atomic/Molecular Massively Parallel Simulator.

LAMMPS is a classical molecular dynamics simulation code designed to run efficiently on parallel computers. It was developed at Sandia National Laboratories, a US Department of Energy facility, with funding from the DOE. It is an open-source code, distributed freely under the terms of the GNU Public License (GPL).

The primary developers of LAMMPS are Steve Plimpton, Aidan Thompson, and Paul Crozier who can be contacted at sjplimp,athomps,pscrozi at sandia.gov. The LAMMPS WWW Site at http://lammps.sandia.gov has more information about the code and its uses.

The LAMMPS documentation is organized into the following sections. If you find errors or omissions in this manual or have suggestions for useful information to add, please send an email to the developers so we can improve the LAMMPS documentation.

Once you are familiar with LAMMPS, you may want to bookmark this page at Section_commands.html#comm since it gives quick access to documentation for all LAMMPS commands.

PDF file of the entire manual, generated by htmldoc

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1. Introduction

This section provides an overview of what LAMMPS can and can't do, describes what it means for LAMMPS to be an open-source code, and acknowledges the funding and people who have contributed to LAMMPS over the years.

1.1 What is LAMMPS
1.2 LAMMPS features
1.3 LAMMPS non-features
1.4 Open source distribution
1.5 Acknowledgments and citations

1.1 What is LAMMPS

LAMMPS is a classical molecular dynamics code that models an ensemble of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, metallic, granular, and coarse-grained systems using a variety of force fields and boundary conditions.

For examples of LAMMPS simulations, see the Publications page of the LAMMPS WWW Site.

LAMMPS runs efficiently on single-processor desktop or laptop machines, but is designed for parallel computers. It will run on any parallel machine that compiles C++ and supports the MPI message-passing library. This includes distributed- or shared-memory parallel machines and Beowulf-style clusters.

LAMMPS can model systems with only a few particles up to millions or billions. See Section_perf for information on LAMMPS performance and scalability, or the Benchmarks section of the LAMMPS WWW Site.

LAMMPS is a freely-available open-source code, distributed under the terms of the GNU Public License, which means you can use or modify the code however you wish. See this section for a brief discussion of the open-source philosophy.

LAMMPS is designed to be easy to modify or extend with new capabilities, such as new force fields, atom types, boundary conditions, or diagnostics. See Section_modify for more details.

The current version of LAMMPS is written in C++. Earlier versions were written in F77 and F90. See Section_history for more information on different versions. All versions can be downloaded from the LAMMPS WWW Site.

LAMMPS was originally developed under a US Department of Energy CRADA (Cooperative Research and Development Agreement) between two DOE labs and 3 companies. It is distributed by Sandia National Labs. See this section for more information on LAMMPS funding and individuals who have contributed to LAMMPS.

In the most general sense, LAMMPS integrates Newton's equations of motion for collections of atoms, molecules, or macroscopic particles that interact via short- or long-range forces with a variety of initial and/or boundary conditions. For computational efficiency LAMMPS uses neighbor lists to keep track of nearby particles. The lists are optimized for systems with particles that are repulsive at short distances, so that the local density of particles never becomes too large. On parallel machines, LAMMPS uses spatial-decomposition techniques to partition the simulation domain into small 3d sub-domains, one of which is assigned to each processor. Processors
communicate and store "ghost" atom information for atoms that border their sub-domain. LAMMPS is most efficient (in a parallel sense) for systems whose particles fill a 3d rectangular box with roughly uniform density. Papers with technical details of the algorithms used in LAMMPS are listed in this section.

1.2 LAMMPS features

This section highlights LAMMPS features, with pointers to specific commands which give more details. If LAMMPS doesn’t have your favorite interatomic potential, boundary condition, or atom type, see Section_modify, which describes how you can add it to LAMMPS.

General features

- runs on a single processor or in parallel
- distributed-memory message-passing parallelism (MPI)
- spatial-decomposition of simulation domain for parallelism
- open-source distribution
- highly portable C++
- optional libraries used: MPI and single-processor FFT
- GPU (CUDA and OpenCL) and OpenMP support for many code features
- easy to extend with new features and functionality
- runs from an input script
- syntax for defining and using variables and formulas
- syntax for looping over runs and breaking out of loops
- run one or multiple simulations simultaneously (in parallel) from one script
- build as library, invoke LAMMPS thru library interface or provided Python wrapper
- couple with other codes: LAMMPS calls other code, other code calls LAMMPS, umbrella code calls both

Particle and model types

(atom style command)

- atoms
- coarse-grained particles (e.g. bead-spring polymers)
- united-atom polymers or organic molecules
- all-atom polymers, organic molecules, proteins, DNA
- metals
- granular materials
- coarse-grained mesoscale models
- finite-size spherical and ellipsoidal particles
- finite-size line segment (2d) and triangle (3d) particles
- point dipolar particles
- rigid collections of particles
- hybrid combinations of these

Force fields

(pair style, bond style, angle style, dihedral style, improper style, kspace style commands)

- pairwise potentials: Lennard-Jones, Buckingham, Morse, Born-Mayer-Huggins, Yukawa, soft, class 2 (COMPASS), hydrogen bond, tabulated
- charged pairwise potentials: Coulombic, point-dipole
manybody potentials: EAM, Finnis/Sinclair EAM, modified EAM (MEAM), embedded ion method (EIM), EDIP, ADP, Stillinger-Weber, Tersoff, REBO, AIREBO, ReaxFF, COMB
• electron force field (eFF, AWPMD)
• coarse-grained potentials: DPD, GayBerne, RESquared, colloidal, DLVO
• mesoscopic potentials: granular, Peridynamics, SPH
• bond potentials: harmonic, FENE, Morse, nonlinear, class 2, quartic (breakable)
• angle potentials: harmonic, CHARMM, cosine, cosine/squared, cosine/periodic, class 2 (COMPASS)
• dihedral potentials: harmonic, CHARMM, multi-harmonic, helix, class 2 (COMPASS), OPLS
• improper potentials: harmonic, cvff, umbrella, class 2 (COMPASS)
• polymer potentials: all-atom, united-atom, bead-spring, breakable
• water potentials: TIP3P, TIP4P, SPC
• implicit solvent potentials: hydrodynamic lubrication, Debye
• KIM archive of potentials
• long-range Coulombics and dispersion: Ewald, Wolf, PPPM (similar to particle-mesh Ewald), Ewald/N for long-range Lennard-Jones
• force-field compatibility with common CHARMM, AMBER, DREIDING, OPLS, GROMACS, COMPASS options
• handful of GPU-enabled pair styles
• hybrid potentials: multiple pair, bond, angle, dihedral, improper potentials can be used in one simulation
• overlaid potentials: superposition of multiple pair potentials

**Atom creation**

(read_data, lattice, create_atoms, delete_atoms, displace_atoms, replicate commands)

• read in atom coords from files
• create atoms on one or more lattices (e.g. grain boundaries)
• delete geometric or logical groups of atoms (e.g. voids)
• replicate existing atoms multiple times
• displace atoms

**Ensembles, constraints, and boundary conditions**

(fix command)

• 2d or 3d systems
• orthogonal or non-orthogonal (triclinic symmetry) simulation domains
• constant NVE, NVT, NPT, NPH, Parinello/Rahman integrators
• thermostating options for groups and geometric regions of atoms
• pressure control via Nose/Hoover or Berendsen barostatting in 1 to 3 dimensions
• simulation box deformation (tensile and shear)
• harmonic (umbrella) constraint forces
• rigid body constraints
• SHAKE bond and angle constraints
• bond breaking, formation, swapping
• walls of various kinds
• non-equilibrium molecular dynamics (NEMD)
• variety of additional boundary conditions and constraints
Integrators

(run, run_style, minimize commands)

- velocity-Verlet integrator
- Brownian dynamics
- rigid body integration
- energy minimization via conjugate gradient or steepest descent relaxation
- rRESPA hierarchical timestepping
- rerun command for post-processing of dump files

Diagnostics

- see the various flavors of the fix and compute commands

Output

(dump, restart commands)

- log file of thermodynamic info
- text dump files of atom coords, velocities, other per-atom quantities
- binary restart files
- parallel I/O of dump and restart files
- per-atom quantities (energy, stress, centro-symmetry parameter, CNA, etc)
- user-defined system-wide (log file) or per-atom (dump file) calculations
- spatial and time averaging of per-atom quantities
- time averaging of system-wide quantities
- atom snapshots in native, XYZ, XTC, DCD, CFG formats

Multi-replica models

nudged elastic band parallel replica dynamics temperature accelerated dynamics parallel tempering

Pre- and post-processing

- Various pre- and post-processing serial tools are packaged with LAMMPS; see these doc pages.
- Our group has also written and released a separate toolkit called Pizza.py which provides tools for doing setup, analysis, plotting, and visualization for LAMMPS simulations. Pizza.py is written in Python and is available for download from the Pizza.py WWW site.

Specialized features

These are LAMMPS capabilities which you may not think of as typical molecular dynamics options:

- stochastic rotation dynamics (SRD)
- real-time visualization and interactive MD
- atom-to-continuum coupling with finite elements
- coupled rigid body integration via the POEMS library
- grand canonical Monte Carlo insertions/deletions
- Direct Simulation Monte Carlo for low-density fluids
- Peridynamics mesoscale modeling
- targeted and steered molecular dynamics
1.3 LAMMPS non-features

LAMMPS is designed to efficiently compute Newton's equations of motion for a system of interacting particles. Many of the tools needed to pre- and post-process the data for such simulations are not included in the LAMMPS kernel for several reasons:

- the desire to keep LAMMPS simple
- they are not parallel operations
- other codes already do them
- limited development resources

Specifically, LAMMPS itself does not:

- run thru a GUI
- build molecular systems
- assign force-field coefficients automagically
- perform sophisticated analyses of your MD simulation
- visualize your MD simulation
- plot your output data

A few tools for pre- and post-processing tasks are provided as part of the LAMMPS package; they are described in this section. However, many people use other codes or write their own tools for these tasks.

As noted above, our group has also written and released a separate toolkit called Pizza.py which addresses some of the listed bullets. It provides tools for doing setup, analysis, plotting, and visualization for LAMMPS simulations. Pizza.py is written in Python and is available for download from the Pizza.py WWW site.

LAMMPS requires as input a list of initial atom coordinates and types, molecular topology information, and force-field coefficients assigned to all atoms and bonds. LAMMPS will not build molecular systems and assign force-field parameters for you.

For atomic systems LAMMPS provides a create_atoms command which places atoms on solid-state lattices (fcc, bcc, user-defined, etc). Assigning small numbers of force field coefficients can be done via the pair coeff, bond coeff, angle coeff, etc commands. For molecular systems or more complicated simulation geometries, users typically use another code as a builder and convert its output to LAMMPS input format, or write their own code to generate atom coordinate and molecular topology for LAMMPS to read in.

For complicated molecular systems (e.g. a protein), a multitude of topology information and hundreds of force-field coefficients must typically be specified. We suggest you use a program like CHARMM or AMBER or other molecular builders to setup such problems and dump its information to a file. You can then reformat the file as LAMMPS input. Some of the tools in this section can assist in this process.

Similarly, LAMMPS creates output files in a simple format. Most users post-process these files with their own analysis tools or re-format them for input into other programs, including visualization packages. If you are convinced you need to compute something on-the-fly as LAMMPS runs, see Section_modify for a discussion of how you can use the dump and compute and fix commands to print out data of your choosing. Keep in mind that complicated computations can slow down the molecular dynamics timestepping, particularly if the computations are not parallel, so it is often better to leave such analysis to post-processing codes.
A very simple (yet fast) visualizer is provided with the LAMMPS package - see the \textit{xmovie} tool in \textit{this section}. It creates xyz projection views of atomic coordinates and animates them. We find it very useful for debugging purposes. For high-quality visualization we recommend the following packages:

- VMD
- AtomEye
- PyMol
- Raster3d
- RasMol

Other features that LAMMPS does not yet (and may never) support are discussed in \textit{Section_history}.

Finally, these are freely-available molecular dynamics codes, most of them parallel, which may be well-suited to the problems you want to model. They can also be used in conjunction with LAMMPS to perform complementary modeling tasks.

- CHARMM
- AMBER
- NAMD
- NWChem
- DL_POLY
- Tinker

CHARMM, AMBER, NAMD, NWChem, and Tinker are designed primarily for modeling biological molecules. CHARMM and AMBER use atom-decomposition (replicated-data) strategies for parallelism; NAMD and NWChem use spatial-decomposition approaches, similar to LAMMPS. Tinker is a serial code. DL_POLY includes potentials for a variety of biological and non-biological materials; both a replicated-data and spatial-decomposition version exist.

1.4 \textbf{Open source distribution}

LAMMPS comes with no warranty of any kind. As each source file states in its header, it is a copyrighted code that is distributed free-of-charge, under the terms of the \textit{GNU Public License} (GPL). This is often referred to as open-source distribution - see \url{www.gnu.org} or \url{www.opensource.org} for more details. The legal text of the GPL is in the LICENSE file that is included in the LAMMPS distribution.

Here is a summary of what the GPL means for LAMMPS users:

(1) Anyone is free to use, modify, or extend LAMMPS in any way they choose, including for commercial purposes.

(2) If you distribute a modified version of LAMMPS, it must remain open-source, meaning you distribute it under the terms of the GPL. You should clearly annotate such a code as a derivative version of LAMMPS.

(3) If you release any code that includes LAMMPS source code, then it must also be open-sourced, meaning you distribute it under the terms of the GPL.

(4) If you give LAMMPS files to someone else, the GPL LICENSE file and source file headers (including the copyright and GPL notices) should remain part of the code.
In the spirit of an open-source code, these are various ways you can contribute to making LAMMPS better. You can send email to the developers on any of these items.

- Point prospective users to the LAMMPS WWW Site. Mention it in talks or link to it from your WWW site.
- If you find an error or omission in this manual or on the LAMMPS WWW Site, or have a suggestion for something to clarify or include, send an email to the developers.
- If you find a bug, Section_errors describes how to report it.
- If you publish a paper using LAMMPS results, send the citation (and any cool pictures or movies if you like) to add to the Publications, Pictures, and Movies pages of the LAMMPS WWW Site, with links and attributions back to you.
- Create a new Makefile.machine that can be added to the src/MAKE directory.
- The tools sub-directory of the LAMMPS distribution has various stand-alone codes for pre- and post-processing of LAMMPS data. More details are given in Section_tools. If you write a new tool that users will find useful, it can be added to the LAMMPS distribution.
- LAMMPS is designed to be easy to extend with new code for features like potentials, boundary conditions, diagnostic computations, etc. This section gives details. If you add a feature of general interest, it can be added to the LAMMPS distribution.
- The Benchmark page of the LAMMPS WWW Site lists LAMMPS performance on various platforms. The files needed to run the benchmarks are part of the LAMMPS distribution. If your machine is sufficiently different from those listed, your timing data can be added to the page.
- You can send feedback for the User Comments page of the LAMMPS WWW Site. It might be added to the page. No promises.
- Cash. Small denominations, unmarked bills preferred. Paper sack OK. Leave on desk. VISA also accepted. Chocolate chip cookies encouraged.

1.5 Acknowledgments and citations

LAMMPS development has been funded by the US Department of Energy (DOE), through its CRADA, LDRD, ASCI, and Genomes-to-Life programs and its OASCR and OBER offices.

Specifically, work on the latest version was funded in part by the US Department of Energy's Genomics:GTL program (www.doegenomestolife.org) under the project, "Carbon Sequestration in Synechococcus Sp.: From Molecular Machines to Hierarchical Modeling".

The following paper describe the basic parallel algorithms used in LAMMPS. If you use LAMMPS results in your published work, please cite this paper and include a pointer to the LAMMPS WWW Site (http://lammps.sandia.gov):


Other papers describing specific algorithms used in LAMMPS are listed under the Citing LAMMPS link of the LAMMPS WWW page.

The Publications link on the LAMMPS WWW page lists papers that have cited LAMMPS. If your paper is not listed there for some reason, feel free to send us the info. If the simulations in your paper produced cool pictures or animations, we'll be pleased to add them to the Pictures or Movies pages of the LAMMPS WWW site.

The core group of LAMMPS developers is at Sandia National Labs:

- Steve Plimpton, sjplimp at sandia.gov
The following folks are responsible for significant contributions to the code, or other aspects of the LAMMPS development effort. Many of the packages they have written are somewhat unique to LAMMPS and the code would not be as general-purpose as it is without their expertise and efforts.

- Axel Kohlmeyer (Temple U), akohlmey at gmail.com, SVN and Git repositories, indefatigable mail list responder, USER-CG-CMM and USER-OMP packages
- Roy Pollock (LLNL), Ewald and PPPM solvers
- Mike Brown (ORNL), brownw at ornl.gov, GPU package
- Greg Wagner (Sandia), gjwagne at sandia.gov, MEAM package for MEAM potential
- Mike Parks (Sandia), mlparks at sandia.gov, PERI package for Peridynamics
- Rudra Mukherjee (JPL), Rudranarayan.M.Mukherjee at jpl.nasa.gov, POEMS package for articulated rigid body motion
- Reese Jones (Sandia) and collaborators, rjones at sandia.gov, USER-ATC package for atom/continuum coupling
- Ilya Valuev (JIHT), valuev at physik.hu-berlin.de, USER-AWPMD package for wave-packet MD
- Christian Trott (U Tech Ilmenau), christian.trott at tu-ilmenau.de, USER-CUDA package
- Andres Jaramillo-Botero (Caltech), ajaramil at wag.caltech.edu, USER-EFF package for electron force field
- Pieter in' t Veld (BASF), pieter.intveld at basf.com, USER-EWALDN package for 1/r^N long-range solvers
- Christoph Kloss (JKU), Christoph.Kloss at jku.at, USER-LIGGHTS package for granular models and granular/liquid coupling
- Metin Aktulga (LBL), hmaktulga at lbl.gov, USER-REAXC package for C version of ReaxFF
- Georg Gunzenmuller (EMI), georg.ganzenmueller at emi.fhg.de, USER-SPH package

As discussed in Section_history, LAMMPS originated as a cooperative project between DOE labs and industrial partners. Folks involved in the design and testing of the original version of LAMMPS were the following:

- John Carpenter (Mayo Clinic, formerly at Cray Research)
- Terry Stouch (Lexicon Pharmaceuticals, formerly at Bristol Myers Squibb)
- Steve Lustig (Dupont)
- Jim Belak (LLNL)
2. Getting Started

This section describes how to build and run LAMMPS, for both new and experienced users.

2.1 What's in the LAMMPS distribution
2.2 Making LAMMPS
2.3 Making LAMMPS with optional packages
2.4 Building LAMMPS via the Make.py script
2.5 Building LAMMPS as a library
2.6 Running LAMMPS
2.7 Command-line options
2.8 Screen output
2.9 Tips for users of previous versions

2.1 What's in the LAMMPS distribution

When you download LAMMPS you will need to unzip and untar the downloaded file with the following commands, after placing the file in an appropriate directory.

```
gunzip lammps*.tar.gz
tar xvf lammps*.tar
```

This will create a LAMMPS directory containing two files and several sub-directories:

<table>
<thead>
<tr>
<th>Directory</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>README</td>
<td>text file</td>
</tr>
<tr>
<td>LICENSE</td>
<td>the GNU General Public License (GPL)</td>
</tr>
<tr>
<td>bench</td>
<td>benchmark problems</td>
</tr>
<tr>
<td>doc</td>
<td>documentation</td>
</tr>
<tr>
<td>examples</td>
<td>simple test problems</td>
</tr>
<tr>
<td>potentials</td>
<td>embedded atom method (EAM) potential files</td>
</tr>
<tr>
<td>src</td>
<td>source files</td>
</tr>
<tr>
<td>tools</td>
<td>pre- and post-processing tools</td>
</tr>
</tbody>
</table>

If you download one of the Windows executables from the download page, then you just get a single file:

```
lmp_windows.exe
```

Skip to the Running LAMMPS sections for info on how to launch these executables on a Windows box.

The Windows executables for serial or parallel only include certain packages and bug-fixes/upgrades listed on this page up to a certain date, as stated on the download page. If you want something with more packages or that is more current, you'll have to download the source tarball and build it yourself from source code using Microsoft Visual Studio, as described in the next section.
2.2 Making LAMMPS

This section has the following sub-sections:

- Read this first
- Steps to build a LAMMPS executable
- Common errors that can occur when making LAMMPS
- Additional build tips
- Building for a Mac
- Building for Windows

Read this first:

Building LAMMPS can be non-trivial. You may need to edit a makefile, there are compiler options to consider, additional libraries can be used (MPI, FFT, JPEG), LAMMPS packages may be included or excluded, some of these packages use auxiliary libraries which need to be pre-built, etc.

Please read this section carefully. If you are not comfortable with makefiles, or building codes on a Unix platform, or running an MPI job on your machine, please find a local expert to help you. Many compiling, linking, and run problems that users have are often not LAMMPS issues - they are peculiar to the user's system, compilers, libraries, etc. Such questions are better answered by a local expert.

If you have a build problem that you are convinced is a LAMMPS issue (e.g. the compiler complains about a line of LAMMPS source code), then please post a question to the LAMMPS mail list.

If you succeed in building LAMMPS on a new kind of machine, for which there isn't a similar Makefile for in the src/MAKE directory, send it to the developers and we can include it in the LAMMPS distribution.

Steps to build a LAMMPS executable:

Step 0

The src directory contains the C++ source and header files for LAMMPS. It also contains a top-level Makefile and a MAKE sub-directory with low-level Makefile.* files for many machines. From within the src directory, type "make" or "gmake". You should see a list of available choices. If one of those is the machine and options you want, you can type a command like:

```make
make linux
or
gmake mac
```

Note that on a multi-processor or multi-core platform you can launch a parallel make, by using the "-j" switch with the make command, which will build LAMMPS more quickly.

If you get no errors and an executable like lmp_linux or lmp_mac is produced, you're done; it's your lucky day.

Note that by default only a few of LAMMPS optional packages are installed. To build LAMMPS with optional packages, see this section below.

Step 1

If Step 0 did not work, you will need to create a low-level Makefile for your machine, like Makefile.foo. You should make a copy of an existing src/MAKE/Makefile.* as a starting point. The only portions of the file you
Step 2

Change the first line of src/MAKE/Makefile.foo to list the word "foo" after the "#", and whatever other options it will set. This is the line you will see if you just type "make".

Step 3

The "compiler/linker settings" section lists compiler and linker settings for your C++ compiler, including optimization flags. You can use g++, the open-source GNU compiler, which is available on all Unix systems. You can also use mpicc which will typically be available if MPI is installed on your system, though you should check which actual compiler it wraps. Vendor compilers often produce faster code. On boxes with Intel CPUs, we suggest using the commercial Intel icc compiler, which can be downloaded from Intel's compiler site.

If building a C++ code on your machine requires additional libraries, then you should list them as part of the LIB variable.

The DEPFLAGS setting is what triggers the C++ compiler to create a dependency list for a source file. This speeds re-compilation when source (*.cpp) or header (*.h) files are edited. Some compilers do not support dependency file creation, or may use a different switch than -D. GNU g++ works with -D. If your compiler can't create dependency files, then you'll need to create a Makefile.foo patterned after Makefile.storm, which uses different rules that do not involve dependency files. Note that when you build LAMMPS for the first time on a new platform, a long list of *.d files will be printed out rapidly. This is not an error; it is the Makefile doing its normal creation of dependencies.

Step 4

The "system-specific settings" section has several parts. Note that if you change any -D setting in this section, you should do a full re-compile, after typing "make clean" (which will describe different clean options).

The LMP_INC variable is used to include options that turn on ifdefs within the LAMMPS code. The options that are currently recognized are:

- DLAMMPS_GZIP
- DLAMMPS_JPEG
- DLAMMPS_MEMALIGN
- DLAMMPS_XDR
- DLAMMPS_SMALLBIG
- DLAMMPS_BIGBIG
- DLAMMPS_SMALLSMALL
- DLAMMPS_LONGLONG_TO_LONG
- DPACK_ARRAY
- DPACK_POINTER
- DPACK_MEMCPY

The read_data and dump commands will read/write gzipped files if you compile with -DLAMMPS_GZIP. It requires that your Unix support the "popen" command.

If you use -DLAMMPS_JPEG, the dump image command will be able to write out JPEG image files. If not, it will only be able to write out text-based PPM image files. For JPEG files, you must also link LAMMPS with a JPEG library, as described below.
Using -DLAMMPS_MEMALIGN= enables the use of the posix_memalign() call instead of malloc() when large chunks or memory are allocated by LAMMPS. This can help to make more efficient use of vector instructions of modern CPUs, since dynamically allocated memory has to be aligned on larger than default byte boundaries (e.g. 16 bytes instead of 8 bytes on x86 type platforms) for optimal performance.

If you use -DLAMMPS_XDR, the build will include XDR compatibility files for doing particle dumps in XTC format. This is only necessary if your platform does have its own XDR files available. See the Restrictions section of the dump command for details.

Use at most one of the -DLAMMPS_SMALLBIG, -DLAMMPS_BIGBIG, -D-DLAMMPS_SMALLSMALL settings. The default is -DLAMMPS_SMALLBIG. These settings refer to use of 4-byte (small) vs 8-byte (big) integers within LAMMPS, as specified in src/lmptype.h. The only reason to use the BIGBIG setting is to enable simulation of huge molecular systems with more than 2 billion atoms or to allow moving atoms to wrap back through a periodic box more than 512 times. The only reason to use the SMALLSMALL setting is if your machine does not support 64-bit integers. See the Additional build tips section below for more details.

The -DLAMMPS_LONGLONG_TO_LONG setting may be needed if your system or MPI version does not recognize "long long" data types. In this case a "long" data type is likely already 64-bits, in which case this setting will convert to that data type.

Using one of the -DPACK_ARRAY, -DPACK_POINTER, and -DPACK_MEMCPY options can make for faster parallel FFTs (in the PPPM solver) on some platforms. The -DPACK_ARRAY setting is the default. See the kspace_style command for info about PPPM. See Step 6 below for info about building LAMMPS with an FFT library.

**Step 5**

The 3 MPI variables are used to specify an MPI library to build LAMMPS with.

If you want LAMMPS to run in parallel, you must have an MPI library installed on your platform. If you use an MPI-wrapped compiler, such as "mpicc" to build LAMMPS, you should be able to leave these 3 variables blank; the MPI wrapper knows where to find the needed files. If not, and MPI is installed on your system in the usual place (under /usr/local), you also may not need to specify these 3 variables. On some large parallel machines which use "modules" for their compile/link environments, you may simply need to include the correct module in your build environment. Or the parallel machine may have a vendor-provided MPI which the compiler has no trouble finding.

Failing this, with these 3 variables you can specify where the mpi.h file (MPI_INC) and the MPI library file (MPI_PATH) are found and the name of the library file (MPI_LIB).

If you are installing MPI yourself, we recommend Argonne's MPICH2 or OpenMPI. MPICH can be downloaded from the Argonne MPI site. OpenMPI can be downloaded from the OpenMPI site. Other MPI packages should also work. If you are running on a big parallel platform, your system people or the vendor should have already installed a version of MPI, which is likely to be faster than a self-installed MPICH or OpenMPI, so find out how to build and link with it. If you use MPICH or OpenMPI, you will have to configure and build it for your platform. The MPI configure script should have compiler options to enable you to use the same compiler you are using for the LAMMPS build, which can avoid problems that can arise when linking LAMMPS to the MPI library.

If you just want to run LAMMPS on a single processor, you can use the dummy MPI library provided in src/STUBS, since you don't need a true MPI library installed on your system. See the src/MAKE/Makefile.serial file for how to specify the 3 MPI variables in this case. You will also need to build the STUBS library for your
platform before making LAMMPS itself. To build from the src directory, type "make stubs", or from the STUBS dir, type "make". This should create a libmpi_stubs.a file suitable for linking to LAMMPS. If the build fails, you will need to edit the STUBS/Makefile for your platform.

The file STUBS/mpi.cpp provides a CPU timer function called MPI_Wtime() that calls gettimeofday(). If your system doesn't support gettimeofday(), you'll need to insert code to call another timer. Note that the ANSI-standard function clock() rolls over after an hour or so, and is therefore insufficient for timing long LAMMPS simulations.

Step 6

The 3 FFT variables allow you to specify an FFT library which LAMMPS uses (for performing 1d FFTs) when running the particle-particle particle-mesh (PPPM) option for long-range Coulombsics via the kspace_style command.

LAMMPS supports various open-source or vendor-supplied FFT libraries for this purpose. If you leave these 3 variables blank, LAMMPS will use the open-source KISS FFT library, which is included in the LAMMPS distribution. This library is portable to all platforms and for typical LAMMPS simulations is almost as fast as FFTW or vendor optimized libraries. If you are not including the KSPACE package in your build, you can also leave the 3 variables blank.

Otherwise, select which kinds of FFTs to use as part of the FFT_INC setting by a switch of the form -DFFT_XXX. Recommended values for XXX are: MKL, SCSL, FFTW2, and FFTW3. Legacy options are: INTEL, SGI, ACML, and T3E. For backward compatibility, using -DFFT_FFTW will use the FFTW2 library. Using -DFFT_NONE will use the KISS library described above.

You may also need to set the FFT_INC, FFT_PATH, and FFT_LIB variables, so the compiler and linker can find the needed FFT header and library files. Note that on some large parallel machines which use "modules" for their compile/link environments, you may simply need to include the correct module in your build environment. Or the parallel machine may have a vendor-provided FFT library which the compiler has no trouble finding.

FFTW is a fast, portable library that should also work on any platform. You can download it from www.fftw.org. Both the legacy version 2.1.X and the newer 3.X versions are supported as -DFFT_FFTW2 or -DFFT_FFTW3. Building FFTW for your box should be as simple as ./configure; make. Note that on some platforms FFTW2 has been pre-installed, and uses renamed files indicating the precision it was compiled with, e.g. sfftw.h, or dfftw.h instead of fftw.h. In this case, you can specify an additional define variable for FFT_INC called -DFFTW_SIZE, which will select the correct include file. In this case, for FFT_LIB you must also manually specify the correct library, namely -lsfftw or -ldfftw.

The FFT_INC variable also allows for a -DFFT_SINGLE setting that will use single-precision FFTs with PPPM, which can speed-up long-range calulations, particularly in parallel or on GPUs. Fourier transform and related PPPM operations are somewhat insensitive to floating point truncation errors and thus do not always need to be performed in double precision. Using the -DFFT_SINGLE setting trades off a little accuracy for reduced memory use and parallel communication costs for transposing 3d FFT data. Note that single precision FFTs have only been tested with the FFTW3, FFTW2, MKL, and KISS FFT options.

Step 7

The 3 JPG variables allow you to specify a JPEG library which LAMMPS uses when writing out JPEG files via the dump image command. These can be left blank if you do not use the -DLAMMPS_JPEG switch discussed above in Step 4, since in that case JPEG output will be disabled.
A standard JPEG library usually goes by the name libjpeg.a and has an associated header file jpeglib.h. Whichever JPEG library you have on your platform, you'll need to set the appropriate JPG_INC, JPG_PATH, and JPG_LIB variables, so that the compiler and linker can find it.

As before, if these header and library files are in the usual place on your machine, you may not need to set these variables.

**Step 8**

Note that by default only a few of LAMMPS optional packages are installed. To build LAMMPS with optional packages, see this section below, before proceeding to Step 9.

**Step 9**

That's it. Once you have a correct Makefile.foo, you have installed the optional LAMMPS packages you want to include in your build, and you have pre-built any other needed libraries (e.g. MPI, FFT, package libraries), all you need to do from the src directory is type something like this:

```
make foo
or
gmake foo
```

You should get the executable lmp_foo when the build is complete.

**Errors that can occur when making LAMMPS:**

IMPORTANT NOTE: If an error occurs when building LAMMPS, the compiler or linker will state very explicitly what the problem is. The error message should give you a hint as to which of the steps above has failed, and what you need to do in order to fix it. Building a code with a Makefile is a very logical process. The compiler and linker need to find the appropriate files and those files need to be compatible with LAMMPS source files. When a make fails, there is usually a very simple reason, which you or a local expert will need to fix.

Here are two non-obvious errors that can occur:

(1) If the make command breaks immediately with errors that indicate it can't find files with a "*" in their names, this can be because your machine's native make doesn't support wildcard expansion in a makefile. Try gmake instead of make. If that doesn't work, try using a -f switch with your make command to use a pre-generated Makefile.list which explicitly lists all the needed files, e.g.

```
make makelist
make -f Makefile.list linux
gmake -f Makefile.list mac
```

The first "make" command will create a current Makefile.list with all the file names in your src dir. The 2nd "make" command (make or gmake) will use it to build LAMMPS. Note that you should include/exclude any desired optional packages before using the "make makelist" command.

(2) If you get an error that says something like 'identifier "atoll" is undefined', then your machine does not support "long long" integers. Try using the -DLAMMPS_LONGLONG_TO_LONG setting described above in Step 4.

**Additional build tips:**

(1) Building LAMMPS for multiple platforms.
You can make LAMMPS for multiple platforms from the same src directory. Each target creates its own object sub-directory called Obj_target where it stores the system-specific *.o files.

(2) Cleaning up.

Typing "make clean-all" or "make clean-foo" will delete *.o object files created when LAMMPS is built, for either all builds or for a particular machine.

(3) Changing the LAMMPS size limits via -DLAMMPS_SMALLBIG or -DLAMMPS_BIBIG or -DLAMMPS_SMALLSMALL

As explained above, any of these 3 settings can be specified on the LMP_INC line in your low-level src/MAKE/Makefile.foo.

The default is -DLAMMPS_SMALLBIG which allows for systems with up to \(2^{63}\) atoms and timesteps (about 9 billion billion). The atom limit is for atomic systems that do not require atom IDs. For molecular models, which require atom IDs, the limit is \(2^{31}\) atoms (about 2 billion). With this setting, image flags are stored in 32-bit integers, which means for 3 dimensions that atoms can only wrap around a periodic box at most 512 times. If atoms move through the periodic box more than this limit, the image flags will "roll over", e.g. from 511 to -512, which can cause diagnostics like the mean-squared displacement, as calculated by the compute msd command, to be faulty.

To allow for larger molecular systems or larger image flags, compile with -DLAMMPS_BIGBIG. This enables molecular systems with up to \(2^{63}\) atoms (about 9 billion billion). And image flags will not "roll over" until they reach \(2^{20} = 1048576\).

IMPORTANT NOTE: As of 6/2012, the BIGBIG setting does not yet enable molecular systems to grow as large as \(2^{63}\). Only the image flag roll over is currently affected by this compile option.

If your system does not support 8-byte integers, you will need to compile with the -DLAMMPS_SMALLSMALL setting. This will restrict your total number of atoms (for atomic or molecular models) and timesteps to \(2^{31}\) (about 2 billion). Image flags will roll over at \(2^{9} = 512\).

Note that in src/lmptype.h there are also settings for the MPI data types associated with the integers that store atom IDs and total system sizes. These need to be consistent with the associated C data types, or else LAMMPS will generate a run-time error.

In all cases, the size of problem that can be run on a per-processor basis is limited by 4-byte integer storage to \(2^{31}\) atoms per processor (about 2 billion). This should not normally be a restriction since such a problem would have a huge per-processor memory footprint due to neighbor lists and would run very slowly in terms of CPU secs/timestep.

Building for a Mac:

OS X is BSD Unix, so it should just work. See the src/MAKE/Makefile.mac file.

Building for Windows:

The LAMMPS download page has an option to download both a serial and parallel pre-built Windows executable. See the Running LAMMPS section for instructions for running these executables on a Windows box.
The pre-built executables are built with a subset of the available packages; see the download page for the list. If you want a Windows version with specific packages included and excluded, you can build it yourself.

One way to do this is install and use cygwin to build LAMMPS with a standard Linux make, just as you would on any Linux box; see src/MAKE/Makefile.cygwin.

The other way to do this is using Visual Studio and project files. See the src/WINDOWS directory and its README.txt file for instructions on both a basic build and a customized build with packages you select.

### 2.3 Making LAMMPS with optional packages

This section has the following sub-sections:

- Package basics
- Including/excluding packages
- Packages that require extra libraries
- Additional Makefile settings for extra libraries

#### Package basics:

The source code for LAMMPS is structured as a set of core files which are always included, plus optional packages. Packages are groups of files that enable a specific set of features. For example, force fields for molecular systems or granular systems are in packages. You can see the list of all packages by typing "make package" from within the src directory of the LAMMPS distribution.

If you use a command in a LAMMPS input script that is specific to a particular package, you must have built LAMMPS with that package, else you will get an error that the style is invalid or the command is unknown. Every command's doc page specifies if it is part of a package. You can also type

```bash
lmp_machine -h
```

to run your executable with the optional `-h` command-line switch for "help", which will list the styles and commands known to your executable.

There are two kinds of packages in LAMMPS, standard and user packages. More information about the contents of standard and user packages is given in Section_packages of the manual. The difference between standard and user packages is as follows:

Standard packages are supported by the LAMMPS developers and are written in a syntax and style consistent with the rest of LAMMPS. This means we will answer questions about them, debug and fix them if necessary, and keep them compatible with future changes to LAMMPS.

User packages have been contributed by users, and always begin with the user prefix. If they are a single command (single file), they are typically in the user-misc package. Otherwise, they are a set of files grouped together which add a specific functionality to the code.

User packages don't necessarily meet the requirements of the standard packages. If you have problems using a feature provided in a user package, you will likely need to contact the contributor directly to get help. Information on how to submit additions you make to LAMMPS as a user-contributed package is given in this section of the documentation.

#### Including/excluding packages:

To use or not use a package you must include or exclude it before building LAMMPS. From the src directory, this is typically as simple as:

```
make yes-colloid
make g++
```

or

```
make no-manybody
make g++
```

Some packages have individual files that depend on other packages being included. LAMMPS checks for this and does the right thing. I.e. individual files are only included if their dependencies are already included. Likewise, if a package is excluded, other files dependent on that package are also excluded.

The reason to exclude packages is if you will never run certain kinds of simulations. For some packages, this will keep you from having to build auxiliary libraries (see below), and will also produce a smaller executable which may run a bit faster.

When you download a LAMMPS tarball, these packages are pre-installed in the src directory: KSPACE, MANYBODY, MOLECULE. When you download LAMMPS source files from the SVN or Git repositories, no packages are pre-installed.

Packages are included or excluded by typing "make yes-name" or "make no-name", where "name" is the name of the package in lower-case, e.g. name = kspace for the KSPACE package or name = user-atc for the USER-ATC package. You can also type "make yes-standard", "make no-standard", "make yes-user", "make no-user", "make yes-all" or "make no-all" to include/exclude various sets of packages. Type "make package" to see the all of the package-related make options.

IMPORTANT NOTE: Inclusion/exclusion of a package works by simply moving files back and forth between the main src directory and sub-directories with the package name (e.g. src/KSPACE, src/USER-ATC), so that the files are seen or not seen when LAMMPS is built. After you have included or excluded a package, you must re-build LAMMPS.

Additional package-related make options exist to help manage LAMMPS files that exist in both the src directory and in package sub-directories. You do not normally need to use these commands unless you are editing LAMMPS files or have downloaded a patch from the LAMMPS WWW site.

Typing "make package-update" will overwrite src files with files from the package sub-directories if the package has been included. It should be used after a patch is installed, since patches only update the files in the package sub-directory, but not the src files. Typing "make package-overwrite" will overwrite files in the package sub-directories with src files.

Typing "make package-status" will show which packages are currently included. Of those that are included, it will list files that are different in the src directory and package sub-directory. Typing "make package-diff" lists all differences between these files. Again, type "make package" to see all of the package-related make options.

---

**Packages that require extra libraries:**

A few of the standard and user packages require additional auxiliary libraries to be compiled first. If you get a LAMMPS build error about a missing library, this is likely the reason. The source code or hooks to these libraries is included in the LAMMPS distribution under the "lib" directory. Look at the lib/README file for a list of these or see Section_packages of the doc pages.
Each lib directory has a README file (e.g. lib/reax/README) with instructions on how to build that library. Typically this is done in this manner:

```
make -f Makefile.g++
```

in the appropriate directory, e.g. in lib/reax. However, some of the libraries do not build this way. Again, see the library README file for details.

If you are building the library, you will need to use a Makefile that is a match for your system. If one of the provided Makefiles is not appropriate for your system you will need to edit or add one. For example, in the case of Fortran-based libraries, your system must have a Fortran compiler, the settings for which will need to be listed in the Makefile.

When you have built one of these libraries, there are 2 things to check:

1. The file libname.a should now exist in lib/name. E.g. lib/reax/libreax.a. This is the library file LAMMPS will link against. One exception is the lib/cuda library which produces the file liblammpscuda.a, because there is already a system library libcuda.a.

2. The file Makefile.lammps should exist in lib/name. E.g. lib/cuda/Makefile.lammps. This file may be auto-generated by the build of the library, or you may need to make a copy of the appropriate provided file (e.g. lib/meam/Makefile.lammps.gfortran). Either way you should insure that the settings in this file are appropriate for your system.

There are typically 3 settings in the Makefile.lammps file (unless some are blank or not needed): a SYSINC, SYSPATH, and SYSLIB setting, specific to this package. These are settings the LAMMPS build will import when compiling the LAMMPS package files (not the library files), and linking to the auxiliary library. They typically list any other system libraries needed to support the package and where to find them. An example is the BLAS and LAPACK libraries needed by the USER-ATC package. Or the system libraries that support calling Fortran from C++, as the MEAM and REAX packages do.

3. One exception to these rules is the lib/linalg directory, which is simply BLAS and LAPACK files used by the USER-ATC package (and possibly other packages in the future). If you do not have these libraries on your system, you can use one of the Makefiles in this directory (which you may need to modify) to build a dummy BLAS and LAPACK library. It can then be included in the lib/atc/Makefile.lammps file as part of the SYSPATH and SYSLIB lines so that LAMMPS will build properly with the USER-ATC package.

Note that if the Makefile.lammps settings are not correct for your box, the LAMMPS build will likely fail.

There are also a few packages, like KIM and USER-MOLFILE, that use additional auxiliary libraries which are not provided with LAMMPS. In these cases, there is no corresponding sub-directory under the lib directory. You are expected to download and install these libraries yourself before building LAMMPS with the package installed, if they are not already on your system.

However there is still a Makefile.lammps file with settings used when building LAMMPS with the package installed, as in (2) above. Is is found in the package directory itself, e.g. src/KIM/Makefile.lammps. This file contains the same 3 settings described above for SYSINC, SYSPATH, and SYSLIB. The Makefile.lammps file contains instructions on how to specify these settings for your system. You need to specify the settings before building LAMMPS with one of those packages installed, else the LAMMPS build will likely fail.
2.4 Building LAMMPS via the Make.py script

The src directory includes a Make.py script, written in Python, which can be used to automate various steps of the build process.

You can run the script from the src directory by typing either:

```
Make.py
python Make.py
```

which will give you info about the tool. For the former to work, you may need to edit the 1st line of the script to point to your local Python. And you may need to insure the script is executable:

```
chmod +x Make.py
```

The following options are supported as switches:

- `-i file1 file2 ...`
- `-p package1 package2 ...`
- `-u package1 package2 ...`
- `-e package1 arg1 arg2 package2 ...`
- `-o dir`
- `-b machine`
- `-s suffix1 suffix2 ...`
- `-l dir`
- `-j N`
- `-h switch1 switch2 ...`

Help on any switch can be listed by using `-h`, e.g.

```
Make.py -h -i -p
```

At a hi-level, these are the kinds of package management and build tasks that can be performed easily, using the Make.py tool:

- install/uninstall packages and build the associated external libs (use `-p` and `-u` and `-e`)
- install packages needed for one or more input scripts (use `-i` and `-p`)
- build LAMMPS, either in the src dir or new dir (use `-b`)
- create a new dir with only the source code needed for one or more input scripts (use `-i` and `-o`)

The last bullet can be useful when you wish to build a stripped-down version of LAMMPS to run a specific script(s). Or when you wish to move the minimal amount of files to another platform for a remote LAMMPS build.

Note that using Make.py is not a substitute for insuring you have a valid src/MAKE/Makefile.foo for your system, or that external library Makefiles in any lib/* directories you use are also valid for your system. But once you have done that, you can use Make.py to quickly include/exclude the packages and external libraries needed by your input scripts.
2.5 Building LAMMPS as a library

LAMMPS can be built as either a static or shared library, which can then be called from another application or a scripting language. See this section for more info on coupling LAMMPS to other codes. See this section for more info on wrapping and running LAMMPS from Python.

Static library:

To build LAMMPS as a static library (*.a file on Linux), type

```
make makelib
make -f Makefile.lib foo
```

where foo is the machine name. This kind of library is typically used to statically link a driver application to LAMMPS, so that you can insure all dependencies are satisfied at compile time. Note that inclusion or exclusion of any desired optional packages should be done before typing "make makelib". The first "make" command will create a current Makefile.lib with all the file names in your src dir. The second "make" command will use it to build LAMMPS as a static library, using the ARCHIVE and ARFLAGS settings in src/MAKE/Makefile.foo. The build will create the file liblammps_foo.a which another application can link to.

Shared library:

To build LAMMPS as a shared library (*.so file on Linux), which can be dynamically loaded, e.g. from Python, type

```
make makeshlib
make -f Makefile.shlib foo
```

where foo is the machine name. This kind of library is required when wrapping LAMMPS with Python; see Section_python for details. Again, note that inclusion or exclusion of any desired optional packages should be done before typing "make makelib". The first "make" command will create a current Makefile.shlib with all the file names in your src dir. The second "make" command will use it to build LAMMPS as a shared library, using the SHFLAGS and SHLIBFLAGS settings in src/MAKE/Makefile.foo. The build will create the file liblammps_foo.so which another application can link to dynamically. It will also create a soft link liblammps.so, which the Python wrapper uses by default.

Note that for a shared library to be usable by a calling program, all the auxiliary libraries it depends on must also exist as shared libraries. This will be the case for libraries included with LAMMPS, such as the dummy MPI library in src/STUBS or any package libraries in lib/packges, since they are always built as shared libraries with the -fPIC switch. However, if a library like MPI or FFTW does not exist as a shared library, the second make command will generate an error. This means you will need to install a shared library version of the package. The build instructions for the library should tell you how to do this.

As an example, here is how to build and install the MPICH library, a popular open-source version of MPI, distributed by Argonne National Labs, as a shared library in the default /usr/local/lib location:

```
./configure --enable-shared
make
make install
```

You may need to use "sudo make install" in place of the last line if you do not have write privileges for /usr/local/lib. The end result should be the file /usr/local/lib/libmpich.so.
Additional requirement for using a shared library:

The operating system finds shared libraries to load at run-time using the environment variable LD_LIBRARY_PATH. So you may wish to copy the file src/liblammps.so or src/liblammps_g++.so (for example) to a place the system can find it by default, such as /usr/local/lib, or you may wish to add the LAMMPS src directory to LD_LIBRARY_PATH, so that the current version of the shared library is always available to programs that use it.

For the csh or tcsh shells, you would add something like this to your ~/.cshrc file:

```
setenv LD_LIBRARY_PATH $LD_LIBRARY_PATH:/home/sjplimp/lammps/src
```

Calling the LAMMPS library:

Either flavor of library (static or shared) allows one or more LAMMPS objects to be instantiated from the calling program.

When used from a C++ program, all of LAMMPS is wrapped in a LAMMPS_NS namespace; you can safely use any of its classes and methods from within the calling code, as needed.

When used from a C or Fortran program or a scripting language like Python, the library has a simple function-style interface, provided in src/library.cpp and src/library.h.

See the sample codes in examples/COUPLE/simple for examples of C++ and C and Fortran codes that invoke LAMMPS thru its library interface. There are other examples as well in the COUPLE directory which are discussed in Section_howto 10 of the manual. See Section_python of the manual for a description of the Python wrapper provided with LAMMPS that operates through the LAMMPS library interface.

The files src/library.cpp and library.h define the C-style API for using LAMMPS as a library. See Section_howto 19 of the manual for a description of the interface and how to extend it for your needs.

### 2.6 Running LAMMPS

By default, LAMMPS runs by reading commands from stdin; e.g. lmp_linux < in.file. This means you first create an input script (e.g. in.file) containing the desired commands. This section describes how input scripts are structured and what commands they contain.

You can test LAMMPS on any of the sample inputs provided in the examples or bench directory. Input scripts are named in.* and sample outputs are named log.*.name.P where name is a machine and P is the number of processors it was run on.

Here is how you might run a standard Lennard-Jones benchmark on a Linux box, using mpirun to launch a parallel job:

```
cd src
make linux
cp lmp_linux ../bench
cd ../bench
mpirun -np 4 lmp_linux <in.lj
```

See this page for timings for this and the other benchmarks on various platforms.

On a Windows box, you can skip making LAMMPS and simply download an executable, as described above, though the pre-packaged executables include only certain packages.
To run a LAMMPS executable on a Windows machine, first decide whether you want to download the non-MPI (serial) or the MPI (parallel) version of the executable. Download and save the version you have chosen.

For the non-MPI version, follow these steps:

• Get a command prompt by going to Start->Run... , then typing "cmd".
• Move to the directory where you have saved lmp_win_no-mpi.exe (e.g. by typing: cd "Documents").
• At the command prompt, type "lmp_win_no-mpi -in in.lj", replacing in.lj with the name of your LAMMPS input script.

For the MPI version, which allows you to run LAMMPS under Windows on multiple processors, follow these steps:

• Download and install MPICH2 for Windows.
• You'll need to use the mpiexec.exe and smpd.exe files from the MPICH2 package. Put them in same directory (or path) as the LAMMPS Windows executable.
• Get a command prompt by going to Start->Run... , then typing "cmd".
• Move to the directory where you have saved lmp_win_mpi.exe (e.g. by typing: cd "Documents").
• Then type something like this: "mpiexec -np 4 -localonly lmp_win_mpi -in in.lj", replacing in.lj with the name of your LAMMPS input script.
• Note that you may need to provide smpd with a passphrase --- it doesn't matter what you type.
• In this mode, output may not immediately show up on the screen, so if your input script takes a long time to execute, you may need to be patient before the output shows up.
• Alternatively, you can still use this executable to run on a single processor by typing something like: "lmp_win_mpi -in in.lj".

The screen output from LAMMPS is described in the next section. As it runs, LAMMPS also writes a log.lammps file with the same information.

Note that this sequence of commands copies the LAMMPS executable (lmp_linux) to the directory with the input files. This may not be necessary, but some versions of MPI reset the working directory to where the executable is, rather than leave it as the directory where you launch mpirun from (if you launch lmp_linux on its own and not under mpirun). If that happens, LAMMPS will look for additional input files and write its output files to the executable directory, rather than your working directory, which is probably not what you want.

If LAMMPS encounters errors in the input script or while running a simulation it will print an ERROR message and stop or a WARNING message and continue. See Section_errors for a discussion of the various kinds of errors LAMMPS can or can't detect, a list of all ERROR and WARNING messages, and what to do about them.

LAMMPS can run a problem on any number of processors, including a single processor. In theory you should get identical answers on any number of processors and on any machine. In practice, numerical round-off can cause slight differences and eventual divergence of molecular dynamics phase space trajectories.

LAMMPS can run as large a problem as will fit in the physical memory of one or more processors. If you run out of memory, you must run on more processors or setup a smaller problem.

2.7 Command-line options

At run time, LAMMPS recognizes several optional command-line switches which may be used in any order. Either the full word or a one-or-two letter abbreviation can be used:

• -c or -cuda
• -e or -echo
• -i or -in
• -h or -help
• -l or -log
• -p or -partition
• -pl or -plog
• -ps or -pscreen
• -r or -reorder
• -sc or -screen
• -sf or -suffix
• -v or -var

For example, lmp_ibm might be launched as follows:

```bash
mpirun -np 16 lmp_ibm -v f tmp.out -l my.log -sc none <in.alloy
mpirun -np 16 lmp_ibm -var f tmp.out -log my.log -screen none <in.alloy
```

Here are the details on the options:

-cuda on/off

Explicitly enable or disable CUDA support, as provided by the USER-CUDA package. If LAMMPS is built with this package, as described above in Section 2.3, then by default LAMMPS will run in CUDA mode. If this switch is set to "off", then it will not, even if it was built with the USER-CUDA package, which means you can run standard LAMMPS or with the GPU package for testing or benchmarking purposes. The only reason to set the switch to "on", is to check if LAMMPS was built with the USER-CUDA package, since an error will be generated if it was not.

-echo style

Set the style of command echoing. The style can be none or screen or log or both. Depending on the style, each command read from the input script will be echoed to the screen and/or logfile. This can be useful to figure out which line of your script is causing an input error. The default value is log. The echo style can also be set by using the echo command in the input script itself.

-in file

Specify a file to use as an input script. This is an optional switch when running LAMMPS in one-partition mode. If it is not specified, LAMMPS reads its input script from stdin - e.g. lmp_linux < in.run. This is a required switch when running LAMMPS in multi-partition mode, since multiple processors cannot all read from stdin.

-help

Print a list of options compiled into this executable for each LAMMPS style (atom_style, fix, compute, pair_style, bond_style, etc). This can help you know if the command you want to use was included via the appropriate package. LAMMPS will print the info and immediately exit if this switch is used.

-log file

Specify a log file for LAMMPS to write status information to. In one-partition mode, if the switch is not used, LAMMPS writes to the file log.lammps. If this switch is used, LAMMPS writes to the specified file. In multi-partition mode, if the switch is not used, a log.lammps file is created with hi-level status information. Each partition also writes to a log.lammps.N file where N is the partition ID. If the switch is specified in multi-partition mode, the hi-level logfile is named "file" and each partition also logs information to a file.N. For both
one-partition and multi-partition mode, if the specified file is "none", then no log files are created. Using a log command in the input script will override this setting. Option -plog will override the name of the partition log files file.N.

-partition 8x2 4 5 ...

Invoke LAMMPS in multi-partition mode. When LAMMPS is run on P processors and this switch is not used, LAMMPS runs in one partition, i.e. all P processors run a single simulation. If this switch is used, the P processors are split into separate partitions and each partition runs its own simulation. The arguments to the switch specify the number of processors in each partition. Arguments of the form MxN mean M partitions, each with N processors. Arguments of the form N mean a single partition with N processors. The sum of processors in all partitions must equal P. Thus the command "-partition 8x2 4 5" has 10 partitions and runs on a total of 25 processors.

Running with multiple partitions can be useful for running multi-replica simulations, where each replica runs on one or a few processors. Note that with MPI installed on a machine (e.g. your desktop), you can run on more (virtual) processors than you have physical processors.

To run multiple independent simulations from one input script, using multiple partitions, see Section howto 4 of the manual. World- and universe-style variables are useful in this context.

-plog file

Specify the base name for the partition log files, so partition N writes log information to file.N. If file is none, then no partition log files are created. This overrides the filename specified in the -log command-line option. This option is useful when working with large numbers of partitions, allowing the partition log files to be suppressed (-plog none) or placed in a sub-directory (-plog replica_files/log.lammps). If this option is not used the log file for partition N is log.lammps.N or whatever is specified by the -log command-line option.

-pscreen file

Specify the base name for the partition screen file, so partition N writes screen information to file.N. If file is none, then no partition screen files are created. This overrides the filename specified in the -screen command-line option. This option is useful when working with large numbers of partitions, allowing the partition screen files to be suppressed (-pscreen none) or placed in a sub-directory (-pscreen replica_files/screen). If this option is not used the screen file for partition N is screen.N or whatever is specified by the -screen command-line option.

-reorder nth N
-reorder custom filename

Reorder the processors in the MPI communicator used to instantiate LAMMPS, in one of several ways. The original MPI communicator ranks all P processors from 0 to P-1. The mapping of these ranks to physical processors is done by MPI before LAMMPS begins. It may be useful in some cases to alter the rank order. E.g. to insure that cores within each node are ranked in a desired order. Or when using the run_style verlet/split command with 2 partitions to insure that a specific Kspace processor (in the 2nd partition) is matched up with a specific set of processors in the 1st partition. See the Section accelerate doc pages for more details.

If the keyword nth is used with a setting N, then it means every Nth processor will be moved to the end of the ranking. This is useful when using the run_style verlet/split command with 2 partitions via the -partition command-line switch. The first set of processors will be in the first partition, the 2nd set in the 2nd partition. The -reorder command-line switch can alter this so that the 1st N procs in the 1st partition and one proc in the 2nd partition will be ordered consecutively, e.g. as the cores on one physical node. This can boost performance. For example, if you use "-reorder nth 4" and "-partition 9 3" and you are running on 12 processors, the processors will
be reordered from

0 1 2 3 4 5 6 7 8 9 10 11

to

0 1 2 4 5 6 8 9 10 3 7 11

so that the processors in each partition will be

0 1 2 4 5 6 8 9 10
3 7 11

See the "processors" command for how to insure processors from each partition could then be grouped optimally for quad-core nodes.

If the keyword is custom", then a file that specifies a permutation of the processor ranks is also specified. The format of the reorder file is as follows. Any number of initial blank or comment lines (starting with a "#" character) can be present. These should be followed by P lines of the form:

I J

where P is the number of processors LAMMPS was launched with. Note that if running in multi-partition mode (see the -partition switch above) P is the total number of processors in all partitions. The I and J values describe a permutation of the P processors. Every I and J should be values from 0 to P-1 inclusive. In the set of P I values, every proc ID should appear exactly once. Ditto for the set of P J values. A single IJ pairing means that the physical processor with rank I in the original MPI communicator will have rank J in the reordered communicator.

Note that rank ordering can also be specified by many MPI implementations, either by environment variables that specify how to order physical processors, or by config files that specify what physical processors to assign to each MPI rank. The -reorder switch simply gives you a portable way to do this without relying on MPI itself. See the processors out command for how to output info on the final assignment of physical processors to the LAMMPS simulation domain.

-screen file

Specify a file for LAMMPS to write its screen information to. In one-partition mode, if the switch is not used, LAMMPS writes to the screen. If this switch is used, LAMMPS writes to the specified file instead and you will see no screen output. In multi-partition mode, if the switch is not used, hi-level status information is written to the screen. Each partition also writes to a screen.N file where N is the partition ID. If the switch is specified in multi-partition mode, the hi-level screen dump is named "file" and each partition also writes screen information to a file.N. For both one-partition and multi-partition mode, if the specified file is "none", then no screen output is performed. Option -pscreen will override the name of the partition screen files file.N.

-suffix style

Use variants of various styles if they exist. The specified style can be opt, omp, gpu, or cuda. These refer to optional packages that LAMMPS can be built with, as described above in Section 2.3. The "opt" style corresponds to the OPT package, the "omp" style to the USER-OMP package, the "gpu" style to the GPU package, and the "cuda" style to the USER-CUDA package.

As an example, all of the packages provide a pair_style lj/cut variant, with style names lj/cut/opt, lj/cut/omp, lj/cut/gpu, or lj/cut/cuda. A variant styles can be specified explicitly in your input script, e.g. pair_style lj/cut/gpu. If the -suffix switch is used, you do not need to modify your input script. The specified suffix (opt,omp,gpu,cuda)
is automatically appended whenever your input script command creates a new atom, pair, fix, compute, or run style. If the variant version does not exist, the standard version is created.

For the GPU package, using this command-line switch also invokes the default GPU settings, as if the command "package gpu force/neigh 0 0 1" were used at the top of your input script. These settings can be changed by using the package gpu command in your script if desired.

For the OMP package, using this command-line switch also invokes the default OMP settings, as if the command "package omp *" were used at the top of your input script. These settings can be changed by using the package omp command in your script if desired.

The suffix command can also set a suffix and it can also turn off/on any suffix setting made via the command line.

-var name value1 value2 ...

Specify a variable that will be defined for substitution purposes when the input script is read. "Name" is the variable name which can be a single character (referenced as $x in the input script) or a full string (referenced as ${abc}). An index-style variable will be created and populated with the subsequent values, e.g. a set of filenames. Using this command-line option is equivalent to putting the line "variable name index value1 value2 ..." at the beginning of the input script. Defining an index variable as a command-line argument overrides any setting for the same index variable in the input script, since index variables cannot be re-defined. See the variable command for more info on defining index and other kinds of variables and this section for more info on using variables in input scripts.

NOTE: Currently, the command-line parser looks for arguments that start with "-" to indicate new switches. Thus you cannot specify multiple variable values if any of them start with a ",", e.g. a negative numeric value. It is OK if the first value starts with a ",", since it is automatically skipped.

2.8 LAMMPS screen output

As LAMMPS reads an input script, it prints information to both the screen and a log file about significant actions it takes to setup a simulation. When the simulation is ready to begin, LAMMPS performs various initializations and prints the amount of memory (in MBytes per processor) that the simulation requires. It also prints details of the initial thermodynamic state of the system. During the run itself, thermodynamic information is printed periodically, every few timesteps. When the run concludes, LAMMPS prints the final thermodynamic state and a total run time for the simulation. It then appends statistics about the CPU time and storage requirements for the simulation. An example set of statistics is shown here:

Loop time of 49.002 on 2 procs for 2004 atoms

Pair time (%) = 35.0495 (71.5267)
Bond time (%) = 0.092046 (0.187841)
Kspce time (%) = 6.42073 (13.103)
Neigh time (%) = 2.73485 (5.5811)
Comm time (%) = 1.50291 (3.06703)
Outpt time (%) = 0.013799 (0.0281601)
Other time (%) = 2.13669 (4.36041)

Nlocal: 1002 ave, 1015 max, 989 min
Histogram: 1 0 0 0 0 0 0 0 0 1
Nghost: 8720 ave, 8724 max, 8716 min
Histogram: 1 0 0 0 0 0 0 0 0 1
Neighs: 354141 ave, 361422 max, 346860 min
Histogram: 1 0 0 0 0 0 0 0 0 1
Total # of neighbors = 708282
Ave neighs/atom = 353.434
Ave special neighs/atom = 2.34032
Number of reneighborings = 42
Dangerous reneighborings = 2

The first section gives the breakdown of the CPU run time (in seconds) into major categories. The second section lists the number of owned atoms (Nlocal), ghost atoms (Nghost), and pair-wise neighbors stored per processor. The max and min values give the spread of these values across processors with a 10-bin histogram showing the distribution. The total number of histogram counts is equal to the number of processors.

The last section gives aggregate statistics for pair-wise neighbors and special neighbors that LAMMPS keeps track of (see the special_bonds command). The number of times neighbor lists were rebuilt during the run is given as well as the number of potentially "dangerous" rebuilds. If atom movement triggered neighbor list rebuilding (see the neigh_modify command), then dangerous reneighborings are those that were triggered on the first timestep atom movement was checked for. If this count is non-zero you may wish to reduce the delay factor to insure no force interactions are missed by atoms moving beyond the neighbor skin distance before a rebuild takes place.

If an energy minimization was performed via the minimize command, additional information is printed, e.g.

Minimization stats:
  E initial, next-to-last, final = -0.895962 -2.94193 -2.94342
  Gradient 2-norm init/final= 1920.78 20.9992
  Gradient inf-norm init/final= 304.283 9.61216
  Iterations = 36
  Force evaluations = 177

The first line lists the initial and final energy, as well as the energy on the next-to-last iteration. The next 2 lines give a measure of the gradient of the energy (force on all atoms). The 2-norm is the "length" of this force vector; the inf-norm is the largest component. The last 2 lines are statistics on how many iterations and force-evaluations the minimizer required. Multiple force evaluations are typically done at each iteration to perform a 1d line minimization in the search direction.

If a kspace_style long-range Coulombics solve was performed during the run (PPPM, Ewald), then additional information is printed, e.g.

FFT time (% of Kspce) = 0.200313 (8.34477)
FFT Gflops 3d 1d-only = 2.31074 9.19989

The first line gives the time spent doing 3d FFTs (4 per timestep) and the fraction it represents of the total KSpace time (listed above). Each 3d FFT requires computation (3 sets of 1d FFTs) and communication (transposes). The total flops performed is 5Nlog_2(N), where N is the number of points in the 3d grid. The FFTs are timed with and without the communication and a Gflop rate is computed. The 3d rate is with communication; the 1d rate is without (just the 1d FFTs). Thus you can estimate what fraction of your FFT time was spent in communication, roughly 75% in the example above.

2.9 Tips for users of previous LAMMPS versions

The current C++ began with a complete rewrite of LAMMPS 2001, which was written in F90. Features of earlier versions of LAMMPS are listed in Section_history. The F90 and F77 versions (2001 and 99) are also freely distributed as open-source codes; check the LAMMPS WWW Site for distribution information if you prefer those versions. The 99 and 2001 versions are no longer under active development; they do not have all the features of C++ LAMMPS.
If you are a previous user of LAMMPS 2001, these are the most significant changes you will notice in C++ LAMMPS:

1. The names and arguments of many input script commands have changed. All commands are now a single word (e.g. read_data instead of read data).

2. All the functionality of LAMMPS 2001 is included in C++ LAMMPS, but you may need to specify the relevant commands in different ways.

3. The format of the data file can be streamlined for some problems. See the read_data command for details. The data file section "Nonbond Coeff" has been renamed to "Pair Coeff" in C++ LAMMPS.

4. Binary restart files written by LAMMPS 2001 cannot be read by C++ LAMMPS with a read_restart command. This is because they were output by F90 which writes in a different binary format than C or C++ writes or reads. Use the restart2data tool provided with LAMMPS 2001 to convert the 2001 restart file to a text data file. Then edit the data file as necessary before using the C++ LAMMPS read_data command to read it in.

5. There are numerous small numerical changes in C++ LAMMPS that mean you will not get identical answers when comparing to a 2001 run. However, your initial thermodynamic energy and MD trajectory should be close if you have setup the problem for both codes the same.
3. Commands

This section describes how a LAMMPS input script is formatted and the input script commands used to define a LAMMPS simulation.

3.1 LAMMPS input script

LAMMPS executes by reading commands from an input script (text file), one line at a time. When the input script ends, LAMMPS exits. Each command causes LAMMPS to take some action. It may set an internal variable, read in a file, or run a simulation. Most commands have default settings, which means you only need to use the command if you wish to change the default.

In many cases, the ordering of commands in an input script is not important. However, the following rules apply:

1) LAMMPS does not read your entire input script and then perform a simulation with all the settings. Rather, the input script is read one line at a time and each command takes effect when it is read. Thus this sequence of commands:

```plaintext
timestep 0.5
run      100
run      100
```

...does something different than this sequence:

```plaintext
run      100
timestep 0.5
run      100
```

In the first case, the specified timestep (0.5 fmsec) is used for two simulations of 100 timesteps each. In the 2nd case, the default timestep (1.0 fmsec) is used for the 1st 100 step simulation and a 0.5 fmsec timestep is used for the 2nd one.

2) Some commands are only valid when they follow other commands. For example, you cannot set the temperature of a group of atoms until atoms have been defined and a group command is used to define which atoms belong to the group.

3) Sometimes command B will use values that can be set by command A. This means command A must precede command B in the input script if it is to have the desired effect. For example, the `read_data` command initializes the system by setting up the simulation box and assigning atoms to processors. If default values are not desired, the `processors` and `boundary` commands need to be used before `read_data` to tell LAMMPS how to map processors to the simulation box.
Many input script errors are detected by LAMMPS and an ERROR or WARNING message is printed. This section gives more information on what errors mean. The documentation for each command lists restrictions on how the command can be used.

### 3.2 Parsing rules

Each non-blank line in the input script is treated as a command. LAMMPS commands are case sensitive. Command names are lower-case, as are specified command arguments. Upper case letters may be used in file names or user-chosen ID strings.

Here is how each line in the input script is parsed by LAMMPS:

1. If the last printable character on the line is a "&" character (with no surrounding quotes), the command is assumed to continue on the next line. The next line is concatenated to the previous line by removing the "&" character and newline. This allows long commands to be continued across two or more lines.

2. All characters from the first "#" character onward are treated as comment and discarded. See an exception in (6). Note that a comment after a trailing "&" character will prevent the command from continuing on the next line. Also note that for multi-line commands a single leading "#" will comment out the entire command.

3. The line is searched repeatedly for $ characters, which indicate variables that are replaced with a text string. See an exception in (6). If the $ is followed by curly brackets, then the variable name is the text inside the curly brackets. If no curly brackets follow the $, then the variable name is the single character immediately following the $. Thus \$\{myTemp\} and \$x refer to variable names "myTemp" and "x". See the variable command for details of how strings are assigned to variables and how they are substituted for in input script commands.

4. The line is broken into "words" separated by whitespace (tabs, spaces). Note that words can thus contain letters, digits, underscores, or punctuation characters.

5. The first word is the command name. All successive words in the line are arguments.

6. If you want text with spaces to be treated as a single argument, it can be enclosed in either double or single quotes. E.g.

```plaintext
print "Volume = \$v"
pri\n
print 'Volume = \$v'
```

The quotes are removed when the single argument is stored internally. See the dump modify format or if commands for examples. A "#" or "$" character that is between quotes will not be treated as a comment indicator in (2) or substituted for as a variable in (3).

IMPORTANT NOTE: If the argument is itself a command that requires a quoted argument (e.g. using a print command as part of an if or run every command), then the double and single quotes can be nested in the usual manner. See the doc pages for those commands for examples. Only one level of nesting is allowed, but that should be sufficient for most use cases.

### 3.3 Input script structure

This section describes the structure of a typical LAMMPS input script. The "examples" directory in the LAMMPS distribution contains many sample input scripts; the corresponding problems are discussed in Section_example, and animated on the [LAMMPS WWW Site](#).
A LAMMPS input script typically has 4 parts:

1. Initialization
2. Atom definition
3. Settings
4. Run a simulation

The last 2 parts can be repeated as many times as desired. I.e. run a simulation, change some settings, run some more, etc. Each of the 4 parts is now described in more detail. Remember that almost all the commands need only be used if a non-default value is desired.

(1) Initialization

Set parameters that need to be defined before atoms are created or read-in from a file.

The relevant commands are units, dimension, newton, processors, boundary, atom_style, atom_modify.

If force-field parameters appear in the files that will be read, these commands tell LAMMPS what kinds of force fields are being used: pair_style, bond_style, angle_style, dihedral_style, improper_style.

(2) Atom definition

There are 3 ways to define atoms in LAMMPS. Read them in from a data or restart file via the read_data or read_restart commands. These files can contain molecular topology information. Or create atoms on a lattice (with no molecular topology), using these commands: lattice, region, create_box, create_atoms. The entire set of atoms can be duplicated to make a larger simulation using the replicate command.

(3) Settings

Once atoms and molecular topology are defined, a variety of settings can be specified: force field coefficients, simulation parameters, output options, etc.

Force field coefficients are set by these commands (they can also be set in the read-in files): pair_coeff, bond_coeff, angle_coeff, dihedral_coeff, improper_coeff, kspace_style, dielectric, special_bonds.

Various simulation parameters are set by these commands: neighbor, neigh_modify, group, timestep, reset_timestep, run_style, min_style, min_modify.

Fixes impose a variety of boundary conditions, time integration, and diagnostic options. The fix command comes in many flavors.

Various computations can be specified for execution during a simulation using the compute, compute_modify, and variable commands.

Output options are set by the thermo, dump, and restart commands.

(4) Run a simulation

A molecular dynamics simulation is run using the run command. Energy minimization (molecular statics) is performed using the minimize command. A parallel tempering (replica-exchange) simulation can be run using the temper command.
3.4 Commands listed by category

This section lists all LAMMPS commands, grouped by category. The next section lists the same commands alphabetically. Note that some style options for some commands are part of specific LAMMPS packages, which means they cannot be used unless the package was included when LAMMPS was built. Not all packages are included in a default LAMMPS build. These dependencies are listed as Restrictions in the command's documentation.

Initialization:

atom_modify, atom_style, boundary, dimension, newton, processors, units

Atom definition:

create_atoms, create_box, lattice, read_data, read_dump, read_restart, region, replicate

Force fields:

angle_coeff, angle_style, bond_coeff, bond_style, dielectric, dihedral_coeff, dihedral_style, improper_coeff, improper_style, kspace_modify, kspace_style, pair_coeff, pair_modify, pair_style, pair_write, special_bonds

Settings:

communicate, group, mass, min_modify, min_style, neigh_modify, neighbor, reset_timestep, run_style, set, timestep, velocity

Fixes:

fix, fix_modify, unfix

Computes:

compute, compute_modify, uncompute

Output:

dump, dump_image, dump_modify, restart, thermo, thermo_modify, thermo_style, undump, write_restart

Actions:

delete_atoms, delete_bonds, displace_atoms, change_box, minimize, neb_prd, rerun, run, temper

Miscellaneous:

clear, echo, if, include, jump, label, log, next, print, shell, variable

3.5 Individual commands

This section lists all LAMMPS commands alphabetically, with a separate listing below of styles within certain commands. The previous section lists the same commands, grouped by category. Note that some style options for some commands are part of specific LAMMPS packages, which means they cannot be used unless the package was included when LAMMPS was built. Not all packages are included in a default LAMMPS build. These
dependencies are listed as Restrictions in the command's documentation.

<table>
<thead>
<tr>
<th>angle_coeff</th>
<th>angle_style</th>
<th>atom_modify</th>
<th>atom_style</th>
<th>balance</th>
<th>bond_coeff</th>
</tr>
</thead>
<tbody>
<tr>
<td>bond_style</td>
<td>boundary</td>
<td>box</td>
<td>change_box</td>
<td>clear</td>
<td>communicate</td>
</tr>
<tr>
<td>compute</td>
<td>compute_mod</td>
<td>create_atoms</td>
<td>create_box</td>
<td>delete_atoms</td>
<td>delete_bonds</td>
</tr>
<tr>
<td>dielectric</td>
<td>dihedral_coef</td>
<td>dihedral_style</td>
<td>dimension</td>
<td>displace_atoms</td>
<td>dump</td>
</tr>
<tr>
<td>dump image</td>
<td>dump_mod</td>
<td>echo</td>
<td>fix</td>
<td>fix_mod</td>
<td>group</td>
</tr>
<tr>
<td>if</td>
<td>improper_coef</td>
<td>improper_style</td>
<td>include</td>
<td>jump</td>
<td>kspace_mod</td>
</tr>
<tr>
<td>kspace_style</td>
<td>label</td>
<td>lattice</td>
<td>log</td>
<td>mass</td>
<td>minimize</td>
</tr>
<tr>
<td>min_mod</td>
<td>min_style</td>
<td>neb</td>
<td>neigh_mod</td>
<td>neighbor</td>
<td>newton</td>
</tr>
<tr>
<td>next</td>
<td>package</td>
<td>pair_coef</td>
<td>pair_mod</td>
<td>pair_style</td>
<td>pair_write</td>
</tr>
<tr>
<td>partition</td>
<td>prd</td>
<td>print</td>
<td>processors</td>
<td>quit</td>
<td>read_data</td>
</tr>
<tr>
<td>read_dump</td>
<td>read_restart</td>
<td>region</td>
<td>replicate</td>
<td>rerun</td>
<td>reset_timestep</td>
</tr>
<tr>
<td>restart</td>
<td>run</td>
<td>run_style</td>
<td>set</td>
<td>shell</td>
<td>special_bonds</td>
</tr>
<tr>
<td>suffix</td>
<td>tad</td>
<td>temper</td>
<td>thermo</td>
<td>thermo_mod</td>
<td>thermo_style</td>
</tr>
<tr>
<td>timestep</td>
<td>uncompute</td>
<td>undump</td>
<td>unfix</td>
<td>units</td>
<td>variable</td>
</tr>
<tr>
<td>velocity</td>
<td>write_restart</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Fix styles

See the `fix` command for one-line descriptions of each style or click on the style itself for a full description:

<table>
<thead>
<tr>
<th>adapt</th>
<th>addforce</th>
<th>append/atoms</th>
<th>aveforce</th>
<th>ave/atom</th>
<th>ave/correlate</th>
<th>ave/histo</th>
<th>ave/spatial</th>
</tr>
</thead>
<tbody>
<tr>
<td>ave/time</td>
<td>balance</td>
<td>bond/break</td>
<td>bond/create</td>
<td>bond/swap</td>
<td>box/relax</td>
<td>deform</td>
<td>deposit</td>
</tr>
<tr>
<td>drag</td>
<td>dt/reset</td>
<td>efield</td>
<td>enforce2d</td>
<td>evaporate</td>
<td>external</td>
<td>freeze</td>
<td>gcmc</td>
</tr>
<tr>
<td>gravity</td>
<td>heat</td>
<td>indent</td>
<td>langevin</td>
<td>lineforce</td>
<td>momentum</td>
<td>move</td>
<td>msst</td>
</tr>
<tr>
<td>neb</td>
<td>nph</td>
<td>nphug</td>
<td>nph/aspHERE</td>
<td>nph/sphere</td>
<td>npt</td>
<td>npt/aspHERE</td>
<td>npt/sphere</td>
</tr>
<tr>
<td>nve</td>
<td>nve/aspHERE</td>
<td>nve/aspHERE/noforce</td>
<td>nve/limit</td>
<td>nve/line</td>
<td>nve/noforce</td>
<td>nve/sphere</td>
<td>nve/tri</td>
</tr>
<tr>
<td>nvt</td>
<td>nvt/aspHERE</td>
<td>nvt/sllod</td>
<td>nvt/sphere</td>
<td>orient/fcc</td>
<td>planeforce</td>
<td>poems</td>
<td>pour</td>
</tr>
<tr>
<td>press/berendsen</td>
<td>print</td>
<td>qeq/comb</td>
<td>reax/bonds</td>
<td>recenter</td>
<td>restrain</td>
<td>rigid</td>
<td>rigid/nph</td>
</tr>
<tr>
<td>rigid/npt</td>
<td>rigid/nve</td>
<td>rigid/nvt</td>
<td>setforce</td>
<td>shake</td>
<td>spring</td>
<td>spring/rg</td>
<td>spring/self</td>
</tr>
<tr>
<td>srclstore/force</td>
<td>store/state</td>
<td>temp/berendsen</td>
<td>temp/rescale</td>
<td>thermal/conductivity</td>
<td>tmd</td>
<td>ttm</td>
<td></td>
</tr>
<tr>
<td>viscosity</td>
<td>viscous</td>
<td>wall/colloid</td>
<td>wall/gran</td>
<td>wall/harmonic</td>
<td>wall/lj126</td>
<td>wall/lj93</td>
<td>wall/piston</td>
</tr>
<tr>
<td>wall/reflect</td>
<td>wall/region</td>
<td>wall/srd</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

These are fix styles contributed by users, which can be used if LAMMPS is built with the appropriate package.

<table>
<thead>
<tr>
<th>addtorque</th>
<th>atc</th>
<th>colvars</th>
<th>IMD</th>
<th>langevin/eff</th>
<th>meso</th>
</tr>
</thead>
<tbody>
<tr>
<td>meso/stationary</td>
<td>nph/eff</td>
<td>npt/eff</td>
<td>nve/eff</td>
<td>nvt/eff</td>
<td>nvt/sllod/eff</td>
</tr>
<tr>
<td>qeq/reax</td>
<td>reax/c/bonds</td>
<td>smd</td>
<td>temp/rescale/eff</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

These are accelerated fix styles, which can be used if LAMMPS is built with the appropriate accelerated package.

<table>
<thead>
<tr>
<th>freeze/cuda</th>
<th>addforce/cuda</th>
<th>aveforce/cuda</th>
<th>enforce2d/cuda</th>
<th>gravity/cuda</th>
<th>gravity/omp</th>
</tr>
</thead>
<tbody>
<tr>
<td>npt/cuda</td>
<td>nve/cuda</td>
<td>nve/sphere/omp</td>
<td>nvt/cuda</td>
<td>qeq/comb/omp</td>
<td>setforce/cuda</td>
</tr>
<tr>
<td>shake/cuda</td>
<td>temp/berendsen/cuda</td>
<td>temp/rescale/cuda</td>
<td>temp/rescale/limit/cuda</td>
<td>viscous/cuda</td>
<td></td>
</tr>
</tbody>
</table>

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**Compute styles**

See the `compute` command for one-line descriptions of each style or click on the style itself for a full description:

<table>
<thead>
<tr>
<th>angle/local</th>
<th>atom/molecule</th>
<th>bond/local</th>
<th>centro/atom</th>
<th>cluster/atom</th>
<th>cna/atom</th>
</tr>
</thead>
<tbody>
<tr>
<td>com</td>
<td>com/molecule</td>
<td>contact/atom</td>
<td>coord/atom</td>
<td>damage/atom</td>
<td>dihedral/local</td>
</tr>
<tr>
<td>displace/atom</td>
<td>erotate/aspHERE</td>
<td>erotate/sphere</td>
<td>erotate/sphere/atom</td>
<td>event/displace</td>
<td>group/group</td>
</tr>
<tr>
<td>gyration</td>
<td>gyration/molecule</td>
<td>heat/flux</td>
<td>improper/local</td>
<td>ke</td>
<td>ke/atom</td>
</tr>
<tr>
<td>msd</td>
<td>msd/molecule</td>
<td>pair</td>
<td>pair/local</td>
<td>pe</td>
<td>pe/atom</td>
</tr>
<tr>
<td>pressure</td>
<td>property/atom</td>
<td>property/local</td>
<td>property/molecule</td>
<td>rdf</td>
<td>reduce</td>
</tr>
<tr>
<td>reduce/region</td>
<td>slice</td>
<td>stress/atom</td>
<td>temp</td>
<td>temp/asphere</td>
<td>temp/com</td>
</tr>
<tr>
<td>temp/deform</td>
<td>temp/partial</td>
<td>temp/profile</td>
<td>temp/ramp</td>
<td>temp/region</td>
<td>temp/sphere</td>
</tr>
<tr>
<td>ti</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

These are compute styles contributed by users, which can be used if LAMMPS is built with the appropriate package.

<table>
<thead>
<tr>
<th>ackland/atom</th>
<th>ke/eff</th>
<th>ke/atom/eff</th>
<th>meso_e/atom</th>
<th>meso_rho/atom</th>
<th>meso_t/atom</th>
</tr>
</thead>
<tbody>
<tr>
<td>temp/eff</td>
<td>temp/deform/eff</td>
<td>temp/region/eff</td>
<td>temp/rotate</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

These are accelerated compute styles, which can be used if LAMMPS is built with the appropriate accelerated package.

**Pair_style potentials**

See the `pair_style` command for an overview of pair potentials. Click on the style itself for a full description:

<table>
<thead>
<tr>
<th>none</th>
<th>hybrid</th>
<th>hybrid/overlay</th>
<th>adp</th>
</tr>
</thead>
<tbody>
<tr>
<td>airebo</td>
<td>beck</td>
<td>bop</td>
<td>born</td>
</tr>
<tr>
<td>born/coul/long</td>
<td>born/coul/wolf</td>
<td>brownian</td>
<td>brownian/poly</td>
</tr>
<tr>
<td>buck</td>
<td>buck/coul/cut</td>
<td>buck/coul/long</td>
<td>colloid</td>
</tr>
<tr>
<td>comb</td>
<td>coul/cut</td>
<td>coul/debye</td>
<td>coul/long</td>
</tr>
<tr>
<td>coul/wolf</td>
<td>dipole/cut</td>
<td>dpd</td>
<td>dpd/tstat</td>
</tr>
<tr>
<td>dsmc</td>
<td>eam</td>
<td>eam/alloy</td>
<td>eam/fs</td>
</tr>
<tr>
<td>eim</td>
<td>gauss</td>
<td>gayberne</td>
<td>gran/hertz/history</td>
</tr>
<tr>
<td>gran/hooke</td>
<td>gran/hooke/history</td>
<td>hbond/dreiding/lj</td>
<td>hbond/dreiding/morse</td>
</tr>
<tr>
<td>kim</td>
<td>lcbop</td>
<td>line/lj</td>
<td>lj/charmmp/coul/charmmp</td>
</tr>
<tr>
<td>lj/charmmp/coul/charmmp/implicit</td>
<td>lj/charmmp/coul/long</td>
<td>lj/class2</td>
<td>lj/class2/coul/cut</td>
</tr>
<tr>
<td>lj/class2/coul/long</td>
<td>lj/cut</td>
<td>lj/cut/coul/cut</td>
<td>lj/cut/coul/debye</td>
</tr>
<tr>
<td>lj/cut/coul/long</td>
<td>lj/cut/coul/long/tip4p</td>
<td>lj/expand</td>
<td>lj/gromacs</td>
</tr>
<tr>
<td>lj/gromacs/coul/gromacs</td>
<td>lj/expand</td>
<td>lj/expand/linear</td>
<td>lj96/cut</td>
</tr>
<tr>
<td>lubricate</td>
<td>lubricate/poly</td>
<td>lubricateU</td>
<td>lubricateU/poly</td>
</tr>
<tr>
<td>meam</td>
<td>morse</td>
<td>peri/lps</td>
<td>peri/pmb</td>
</tr>
<tr>
<td>reax</td>
<td>rebo</td>
<td>resquared</td>
<td>soft</td>
</tr>
<tr>
<td>sw</td>
<td>table</td>
<td>tersoff</td>
<td>tersoff/zbl</td>
</tr>
</tbody>
</table>
These are pair styles contributed by users, which can be used if LAMMPS is built with the appropriate package.

<table>
<thead>
<tr>
<th>tri/lj</th>
<th>yukawa</th>
<th>yukawa/colloid</th>
</tr>
</thead>
</table>

These are accelerated pair styles, which can be used if LAMMPS is built with the appropriate accelerated package.

<table>
<thead>
<tr>
<th>adp/omp</th>
<th>airebo/omp</th>
<th>beck/omp</th>
<th>born/coul/long/cuda</th>
</tr>
</thead>
<tbody>
<tr>
<td>born/coul/long/omp</td>
<td>born/coul/wolf/omp</td>
<td>born/omp</td>
<td>brownian/omp</td>
</tr>
<tr>
<td>brownian/poly/omp</td>
<td>buck/coul/cut/cuda</td>
<td>buck/coul/cut/gpu</td>
<td>buck/coul/cut/omp</td>
</tr>
<tr>
<td>buck/coul/long/cuda</td>
<td>buck/coul/long/gpu</td>
<td>buck/coul/long/omp</td>
<td>buck/coul/omp</td>
</tr>
<tr>
<td>buck/cuda</td>
<td>buck/gpu</td>
<td>buck/omp</td>
<td>colloid/omp</td>
</tr>
<tr>
<td>comb/omp</td>
<td>coul/cut/omp</td>
<td>coul/debye/omp</td>
<td>coul/long/gpu</td>
</tr>
<tr>
<td>coul/long/omp</td>
<td>coul/wolf</td>
<td>dipole/cut/omp</td>
<td>dipole/sf/omp</td>
</tr>
<tr>
<td>dpd/omp</td>
<td>dpd/tstat/omp</td>
<td>eam/alloy/cuda</td>
<td>eam/cuda</td>
</tr>
<tr>
<td>eam/alloy/omp</td>
<td>eam/alloy/opt</td>
<td>eam/cd/omp</td>
<td>eam/cuda</td>
</tr>
<tr>
<td>eam/fs/omp</td>
<td>eam/fs/gpu</td>
<td>eam/fs/omp</td>
<td>eam/fs/opt</td>
</tr>
<tr>
<td>eam/gpu</td>
<td>eam/omp</td>
<td>eam/omp</td>
<td>edip/omp</td>
</tr>
<tr>
<td>eim/omp</td>
<td>gauss/omp</td>
<td>gayberne/gpu</td>
<td>gayberne/omp</td>
</tr>
<tr>
<td>gran/hertz/history/omp</td>
<td>gran/hooke/cuda</td>
<td>gran/hooke/history/omp</td>
<td>gran/hooke/omp</td>
</tr>
</tbody>
</table>

| lj/charm/coul/long/gpu | lj/charm/coul/long/omp | lj/charm/coul/long/opt | lj/charm/coul/long/pppm/omp |
| lj/class2/coul/cut/cuda | lj/class2/coul/cut/omp | lj/class2/coul/long/gpu | lj/class2/coul/long/pcm/omp |
| lj/class2/coul/pppm/omp | lj/class2/coul/long/omp | lj/class2/coul/long/pcm/omp | lj/class2/coul/long/pcm/omp |
| lj/class2/omp | lj/coul/omp | lj/coul/cut/cuda | lj/coul/cut/gpu |
| lj/cut/coul/cut/omp | lj/coul/coul/debye/omp | lj/coul/coul/debye/omp | lj/coul/coul/long/omp |
| lj/cut/coul/long/gpu | lj/coul/coul/long/omp | lj/coul/coul/long/omp | lj/coul/coul/long/pcm/omp |
| lj/cut/coul/long/tip4p/omp | lj/cut/coul/pppm/omp | lj/cut/coul/pppm/5p/omp | lj/cut/omp |
| lj/cut/experimental/cuda | lj/cut/gpu | lj/cut/omp | lj/cut/omp |
| lj/expand/cuda | lj/expand/gpu | lj/expand/omp | lj/expand/omp |
| lj/gromacs/coul/gromacs/omp | lj/gromacs/coul/gromacs/omp | lj/gromacs/coul/gromacs/omp | lj/gromacs/coul/gromacs/omp |
| lj/sdks/coul | lj/sdks/coul/long/gpu | lj/sdks/coul/long/omp | lj/sdks/gpu |
| lj/smooth/coul | lj/smooth/omp | lj/smooth/linear/omp | lj/96/coul/gpu |
| lj96/coul/gpu | lj96/coul/omp | lubricate/omp | lubricate/poly/omp |
| mean/spline/omp | morse/coul | morse/gpu | morse/omp |
| morse/omp | peri/lps/omp | peri/pmb/omp | rebo/omp |
| resquared/gpu | resquared/omp | soft/omp | sw/cuda |
| sw/omp | table/omp | table/omp | tersoff/cuda |
Bond_style potentials

See the bond_style command for an overview of bond potentials. Click on the style itself for a full description:

<table>
<thead>
<tr>
<th>none</th>
<th>hybrid</th>
<th>class2</th>
<th>fene</th>
</tr>
</thead>
<tbody>
<tr>
<td>fene/expand</td>
<td>harmonic</td>
<td>morse</td>
<td>nonlinear</td>
</tr>
<tr>
<td>quartic</td>
<td>table</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

These are bond styles contributed by users, which can be used if LAMMPS is built with the appropriate package.

| harmonic/shift | harmonic/shift/cut |

These are accelerated bond styles, which can be used if LAMMPS is built with the appropriate accelerated package.

<table>
<thead>
<tr>
<th>class2/omp</th>
<th>fene/omp</th>
<th>fene/expand/omp</th>
<th>harmonic/omp</th>
</tr>
</thead>
<tbody>
<tr>
<td>harmonic/shift/omp</td>
<td>harmonic/shift/cut/omp</td>
<td>morse/omp</td>
<td>nonlinear/omp</td>
</tr>
<tr>
<td>quartic/omp</td>
<td>table/omp</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Angle_style potentials

See the angle_style command for an overview of angle potentials. Click on the style itself for a full description:

<table>
<thead>
<tr>
<th>none</th>
<th>hybrid</th>
<th>charmm</th>
<th>class2</th>
</tr>
</thead>
<tbody>
<tr>
<td>cosine</td>
<td>cosine/delta</td>
<td>cosine/periodic</td>
<td>cosine/squared</td>
</tr>
<tr>
<td>harmonic</td>
<td>table</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

These are angle styles contributed by users, which can be used if LAMMPS is built with the appropriate package.

| sdk | cosine/shift | cosine/shift/exp | dipole |

These are accelerated angle styles, which can be used if LAMMPS is built with the appropriate accelerated package.

<table>
<thead>
<tr>
<th>charmm/omp</th>
<th>class2/omp</th>
<th>cosine/omp</th>
<th>cosine/delta/omp</th>
</tr>
</thead>
<tbody>
<tr>
<td>cosine/periodic/omp</td>
<td>cosine/shift/omp</td>
<td>cosine/shift/exp/omp</td>
<td>cosine/squared/omp</td>
</tr>
<tr>
<td>dipole/ompharmonic/omp</td>
<td>table/omp</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Dihedral_style potentials

See the dihedral_style command for an overview of dihedral potentials. Click on the style itself for a full description:

<table>
<thead>
<tr>
<th>none</th>
<th>hybrid</th>
<th>charmm</th>
<th>class2</th>
</tr>
</thead>
<tbody>
<tr>
<td>harmonic</td>
<td>helix</td>
<td>multi/harmonic</td>
<td>opls</td>
</tr>
</tbody>
</table>

These are dihedral styles contributed by users, which can be used if LAMMPS is built with the appropriate package.

| cosine/shift/exp | table |

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These are accelerated dihedral styles, which can be used if LAMMPS is built with the appropriate accelerated package.

<table>
<thead>
<tr>
<th>charmm/omp</th>
<th>class2/omp</th>
<th>cosine/shift/exp/omp</th>
<th>harmonic/omp</th>
</tr>
</thead>
<tbody>
<tr>
<td>helix/omp</td>
<td>multi/harmonic/omp</td>
<td>opls/omptable/omp</td>
<td></td>
</tr>
</tbody>
</table>

**Improper_style potentials**

See the improper_style command for an overview of improper potentials. Click on the style itself for a full description:

<table>
<thead>
<tr>
<th>none</th>
<th>hybrid</th>
<th>class2</th>
<th>cvff</th>
</tr>
</thead>
<tbody>
<tr>
<td>harmonic</td>
<td>umbrella</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

These are improper styles contributed by users, which can be used if LAMMPS is built with the appropriate package.

| cossq        | ring        |

These are accelerated improper styles, which can be used if LAMMPS is built with the appropriate accelerated package.

<table>
<thead>
<tr>
<th>class2/omp</th>
<th>cossq/omp</th>
<th>cvff/omp</th>
<th>harmonic/omp</th>
</tr>
</thead>
<tbody>
<tr>
<td>ring/omp</td>
<td>umbrella/omp</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Kspace solvers**

See the kspace_style command for an overview of Kspace solvers. Click on the style itself for a full description:

| ewald        | pppm        | pppm/cg     | pppm/tip4p  |

These are Kspace solvers contributed by users, which can be used if LAMMPS is built with the appropriate package.

| ewald/n      |             |

These are accelerated Kspace solvers, which can be used if LAMMPS is built with the appropriate accelerated package.

<table>
<thead>
<tr>
<th>ewald/omp</th>
<th>pppm/cuda</th>
<th>pppm/gpu</th>
<th>pppm/omp</th>
</tr>
</thead>
<tbody>
<tr>
<td>pppm/cg/omp</td>
<td>pppm/tip4p/omp</td>
<td>pppm/proxy</td>
<td>pppm/tip4p/proxy</td>
</tr>
</tbody>
</table>
4. Packages

This section gives a quick overview of the add-on packages that extend LAMMPS functionality.

4.1 Standard packages
4.2 User packages

LAMMPS includes many optional packages, which are groups of files that enable a specific set of features. For example, force fields for molecular systems or granular systems are in packages. You can see the list of all packages by typing "make package" from within the src directory of the LAMMPS distribution.

See Section_start 3 of the manual for details on how to include/exclude specific packages as part of the LAMMPS build process, and for more details about the differences between standard packages and user packages in LAMMPS.

Below, the packages currently available in LAMMPS are listed. For standard packages, just a one-line description is given. For user packages, more details are provided.

### 4.1 Standard packages

The current list of standard packages is as follows:

<table>
<thead>
<tr>
<th>Package</th>
<th>Description</th>
<th>Author(s)</th>
<th>Doc page</th>
<th>Example</th>
<th>Library</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASPHERE</td>
<td>aspherical particles</td>
<td>-</td>
<td>Section_howto</td>
<td>ellipse</td>
<td>-</td>
</tr>
<tr>
<td>CLASS2</td>
<td>class 2 force fields</td>
<td>-</td>
<td>pair_style lj/class2</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>COLLOID</td>
<td>colloidal particles</td>
<td>-</td>
<td>atom_style colloid</td>
<td>colloid</td>
<td>-</td>
</tr>
<tr>
<td>DIPOLE</td>
<td>point dipole particles</td>
<td>-</td>
<td>pair_style dipole/cut</td>
<td>dipole</td>
<td>-</td>
</tr>
<tr>
<td>FLD</td>
<td>Fast Lubrication Dynamics</td>
<td>Kumar &amp; Bybee &amp; Higdon (1)</td>
<td>pair_style lubricateU</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>GPU</td>
<td>GPU-enabled potentials</td>
<td>Mike Brown (ORNL)</td>
<td>Section_accelerate</td>
<td>gpu</td>
<td>lib/gpu</td>
</tr>
<tr>
<td>GRANULAR</td>
<td>granular systems</td>
<td>-</td>
<td>Section_howto</td>
<td>pour</td>
<td>-</td>
</tr>
<tr>
<td>KIM</td>
<td>openKIM potentials</td>
<td>Smirichinski &amp; Elliot &amp; Tadmor (3)</td>
<td>pair_style kim</td>
<td>kim</td>
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</tr>
<tr>
<td>KSPACE</td>
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<td>MANYBODY</td>
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<td>MEAM</td>
<td>modified EAM potential</td>
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<td>pair_style meam</td>
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</tr>
<tr>
<td>MC</td>
<td>Monte Carlo options</td>
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</tr>
<tr>
<td>MOLECULE</td>
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</tr>
<tr>
<td>OPT</td>
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</tr>
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<td>PERI</td>
<td>Peridynamics models</td>
<td>Mike Parks (Sandia)</td>
<td>pair_style peri</td>
<td>peri</td>
<td>-</td>
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<tr>
<td>POEMS</td>
<td>-</td>
<td>Rudra Mukherjee (JPL)</td>
<td>fix poems</td>
<td>rigid</td>
<td>lib/poems</td>
</tr>
</tbody>
</table>
The "Authors" column lists a name(s) if a specific person is responsible for creating and maintaining the package.

(1) The FLD package was created by Amit Kumar and Michael Bybee from Jonathan Higdon's group at UIUC.

(2) The OPT package was created by James Fischer (High Performance Technologies), David Richie, and Vincent Natoli (Stone Ridge Technology).

(3) The KIM package was created by Valeriu Smirichinski, Ryan Elliott, and Ellad Tadmor (U Minn).

The "Doc page" column links to either a portion of the Section_howto of the manual, or an input script command implemented as part of the package.

The "Example" column is a sub-directory in the examples directory of the distribution which has an input script that uses the package. E.g. "peptide" refers to the examples/peptide directory.

The "Library" column lists an external library which must be built first and which LAMMPS links to when it is built. These are in the lib directory of the distribution. This section of the manual gives details on the 2-step build process with external libraries.

4.2 User packages

The current list of user-contributed packages is as follows:

<table>
<thead>
<tr>
<th>Package</th>
<th>Description</th>
<th>Author(s)</th>
<th>Doc page</th>
<th>Example</th>
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<td>single-file contributions</td>
<td>USER-MISC/README</td>
<td>USER-MISC/README</td>
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</tr>
<tr>
<td>USER-ATC</td>
<td>atom-to-continuum coupling</td>
<td>Jones &amp; Templeton &amp; Zimmerman (2)</td>
<td>fix atc</td>
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<td>USER-AWPMD</td>
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<td>Ilya Valuev (JIHT)</td>
<td>pair_style awpmd/cut</td>
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<td>lib/awpmd</td>
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<tr>
<td>USER-CG-CMM</td>
<td>coarse-graining model</td>
<td>Axel Kohlmeyer (Temple U)</td>
<td>pair_style lj/sdk</td>
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<td>cg</td>
<td>-</td>
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<tr>
<td>USER-COLVARS</td>
<td>collective variables</td>
<td>Fiorin &amp; Henin &amp; Kohlmeyer (3)</td>
<td>fix colvars</td>
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<td>USER-CUDA</td>
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<td>electron force field</td>
<td>Andres Jaramillo-Botero (Caltech)</td>
<td>pair_style eff/cut</td>
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</tr>
<tr>
<td>USER-EWALDN</td>
<td>Ewald for I/R^n</td>
<td>Pieter in' t Veld (BASF)</td>
<td>kspace_style</td>
<td>-</td>
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</tr>
<tr>
<td>USER-MOLFILE</td>
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<td></td>
<td>dump molfile</td>
<td>-</td>
<td>-</td>
<td>lib/molfile</td>
</tr>
<tr>
<td>Package</td>
<td>Description</td>
<td>Author</td>
<td>Doc Page</td>
<td>Example</td>
<td>Library</td>
<td></td>
</tr>
<tr>
<td>---------</td>
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</tr>
<tr>
<td>USER-OMP</td>
<td>OpenMP threaded styles</td>
<td>Axel Kohlmeyer (Temple U)</td>
<td>Section accelerate</td>
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<td></td>
</tr>
<tr>
<td>USER-REAXC</td>
<td>C version of ReaxFF</td>
<td>Metin Aktulga (LBNL)</td>
<td>pair_style reaxe</td>
<td>reax</td>
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<td></td>
</tr>
<tr>
<td>USER-SPH</td>
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<td>Georg Ganzenmuller (EMI)</td>
<td>userguide.pdf</td>
<td>USER/sph</td>
<td>sph</td>
<td></td>
</tr>
</tbody>
</table>

The "Authors" column lists a name(s) if a specific person is responsible for creating and maintaining the package.

(2) The ATC package was created by Reese Jones, Jeremy Templeton, and Jon Zimmerman (Sandia).

(3) The COLVARS package was created by Axel Kohlmeyer (Temple U) using the colvars module library written by Giacomo Fiorin (Temple U) and Jerome Henin (LISM, Marseille, France).

The "Doc page" column links to either a portion of the Section_howto of the manual, or an input script command implemented as part of the package, or to additional documentation provided with the package.

The "Example" column is a sub-directory in the examples directory of the distribution which has an input script that uses the package. E.g. "peptide" refers to the examples/peptide directory. USER/cuda refers to the examples/USER/cuda directory.

The "Library" column lists an external library which must be built first and which LAMMPS links to when it is built. These are in the lib directory of the distribution. This section of the manual gives details on the 2-step build process with external libraries.

More details on each package, from the USER-blah/README file is given below.

**USER-MISC package**

The files in this package are a potpourri of (mostly) unrelated features contributed to LAMMPS by users. Each feature is a single pair of files (*.cpp and *.h).

More information about each feature can be found by reading its doc page in the LAMMPS doc directory. The doc page which lists all LAMMPS input script commands is as follows:

Section_commands

User-contributed features are listed at the bottom of the fix, compute, pair, etc sections.

The list of features and author of each is given in the src/USER-MISC/README file.

You should contact the author directly if you have specific questions about the feature or its coding.

**USER-ATC package**

This package implements a "fix atc" command which can be used in a LAMMPS input script. This fix can be employed to either do concurrent coupling of MD with FE-based physics surrogates or on-the-fly post-processing of atomic information to continuum fields.
See the doc page for the fix atc command to get started. At the bottom of the doc page are many links to additional documentation contained in the doc/USER/atc directory.

There are example scripts for using this package in examples/USER/atc.

This package uses an external library in lib/atc which must be compiled before making LAMMPS. See the lib/atc/README file and the LAMMPS manual for information on building LAMMPS with external libraries.

The primary people who created this package are Reese Jones (rjones at sandia.gov), Jeremy Templeton (jatempl at sandia.gov) and Jon Zimmerman (jzimmer at sandia.gov) at Sandia. Contact them directly if you have questions.

---

**USER-AWPMD package**

This package contains a LAMMPS implementation of the Antisymmetrized Wave Packet Molecular Dynamics (AWPMD) method.

See the doc page for the pair_style awpmd/cut command to get started.

There are example scripts for using this package in examples/USER/awpmd.

This package uses an external library in lib/awpmd which must be compiled before making LAMMPS. See the lib/awpmd/README file and the LAMMPS manual for information on building LAMMPS with external libraries.

The person who created this package is Ilya Valuev at the JIHT in Russia (valuev at physik.hu-berlin.de). Contact him directly if you have questions.

---

**USER-COLVARS package**

This package implements the "fix colvars" command which can be used in a LAMMPS input script.

This fix allows to use "collective variables" to implement Adaptive Biasing Force, Metadynamics, Steered MD, Umbrella Sampling and Restraints. This code consists of two parts:

- A portable collective variable module library written and maintained by Giacomo Fiorin (ICMS, Temple University, Philadelphia, PA, USA) and Jerome Henin (LISM, CNRS, Marseille, France). This code is located in the directory lib/colvars and needs to be compiled first.
- The colvars fix and an interface layer, exchanges information between LAMMPS and the collective variable module.

See the doc page of fix colvars for more details.

There are example scripts for using this package in examples/USER/colvars

This is a very new interface that does not yet support all features in the module and will see future optimizations and improvements. The colvars module library is also available in NAMD has been thoroughly used and tested there. Bugs and problems are likely due to the interface layers code. Thus the current version of this package should be considered beta quality.

The person who created this package is Axel Kohlmeyer at Temple U (akohlmey at gmail.com). Contact him directly if you have questions.
USER-CG-CMM package

This package implements 3 commands which can be used in a LAMMPS input script:

- pair_style lj/sdk
- pair_style lj/sdk/coul/long
- angle_style sdk

These styles allow coarse grained MD simulations with the parametrization of Shinoda, DeVane, Klein, Mol Sim, 33, 27 (2007) (SDK), with extensions to simulate ionic liquids, electrolytes, lipids and charged amino acids.

See the doc pages for these commands for details.

There are example scripts for using this package in examples/USER/cg-cmm.

This is the second generation implementation reducing the the clutter of the previous version. For many systems with electrostatics, it will be faster to use pair_style hybrid/overlay with lj/sdk and coul/long instead of the combined lj/sdk/coul/long style. since the number of charged atom types is usually small. For any other coulomb interactions this is now required. To exploit this property, the use of the kspace_style pppm/cg is recommended over regular pppm. For all new styles, input file backward compatibility is provided. The old implementation is still available through appending the /old suffix. These will be discontinued and removed after the new implementation has been fully validated.

The current version of this package should be considered beta quality. The CG potentials work correctly for "normal" situations, but have not been testing with all kinds of potential parameters and simulation systems.

The person who created this package is Axel Kohlmeyer at Temple U (akohlmey at gmail.com). Contact him directly if you have questions.

USER-CUDA package

This package provides acceleration of various LAMMPS pair styles, fix styles, compute styles, and long-range Coulombics via PPPM for NVIDIA GPUs.

See this section of the manual to get started:

Section_accelerate

There are example scripts for using this package in examples/USER/cuda.

This package uses an external library in lib/cuda which must be compiled before making LAMMPS. See the lib/cuda/README file and the LAMMPS manual for information on building LAMMPS with external libraries.

The person who created this package is Christian Trott at the University of Technology Ilmenau, Germany (christian.trott at tu-ilmenau.de). Contact him directly if you have questions.

USER-EFF package

This package contains a LAMMPS implementation of the electron Force Field (eFF) currently under development at Caltech, as described in A. Jaramillo-Botero, J. Su, Q. An, and W.A. Goddard III, JCC, 2010. The eFF potential was first introduced by Su and Goddard, in 2007.
EFF can be viewed as an approximation to QM wave packet dynamics and Fermionic molecular dynamics, combining the ability of electronic structure methods to describe atomic structure, bonding, and chemistry in materials, and of plasma methods to describe nonequilibrium dynamics of large systems with a large number of highly excited electrons. We classify it as a mixed QM-classical approach rather than a conventional force field method, which introduces QM-based terms (a spin-dependent repulsion term to account for the Pauli exclusion principle and the electron wavefunction kinetic energy associated with the Heisenberg principle) that reduce, along with classical electrostatic terms between nuclei and electrons, to the sum of a set of effective pairwise potentials. This makes EFF uniquely suited to simulate materials over a wide range of temperatures and pressures where electronically excited and ionized states of matter can occur and coexist.

The necessary customizations to the LAMMPS core are in place to enable the correct handling of explicit electron properties during minimization and dynamics.

See the doc page for the pair_style eff/cut command to get started.

There are example scripts for using this package in examples/USER/eff.

There are auxiliary tools for using this package in tools/eff.

The person who created this package is Andres Jaramillo-Botero at CalTech (ajaramil at wag.caltech.edu). Contact him directly if you have questions.

**USER-EWALDN package**

This package implements 3 commands which can be used in a LAMMPS input script: pair_style lj/coul, pair_style buck/coul, and kspace_style ewald/n.

The "kspace_style ewald/n" command is similar to standard Ewald for charges, but also enables the Lennard-Jones interaction, or any 1/r^N interaction to be of infinite extent, instead of being cutoff. LAMMPS pair potentials for long-range Coulombic interactions, such as lj/cut/coul/long can be used with ewald/n. The two new pair_style commands provide the modifications for the short-range LJ and Buckingham interactions that can also be used with ewald/n.

Two other advantages of kspace_style ewald/n are that

a) it can be used with non-orthogonal (triclinic symmetry) simulation boxes

b) it can include long-range summations not just for Coulombic interactions (1/r), but also for dispersion interactions (1/r^6) and dipole interactions (1/r^3).

Neither of these options is currently possible for other kspace styles such as PPPM and ewald.

See the doc pages for these commands for details.

The person who created these files is Pieter in’ t Veld while at Sandia. He is now at BASF (pieter.intveld at basf.com). Contact him directly if you have questions.

**USER-OMP package**

This package provides OpenMP multi-threading support and other optimizations of various LAMMPS pair styles, dihedral styles, and fix styles.
See this section of the manual to get started:

**Section_accelerate**

The person who created this package is Axel Kohlmeyer at Temple U (akohlmey at gmail.com). Contact him directly if you have questions.

**USER-REAXC package**

This package contains a implementation for LAMMPS of the ReaxFF force field. ReaxFF uses distance-dependent bond-order functions to represent the contributions of chemical bonding to the potential energy. It was originally developed by Adri van Duin and the Goddard group at CalTech.

The USER-REAXC version of ReaxFF (pair_style reax/c), implemented in C, should give identical or very similar results to pair_style reax, which is a ReaxFF implementation on top of a Fortran library, a version of which library was originally authored by Adri van Duin.

The reax/c version should be somewhat faster and more scalable, particularly with respect to the charge equilibration calculation. It should also be easier to build and use since there are no complicating issues with Fortran memory allocation or linking to a Fortran library.

For technical details about this implemenation of ReaxFF, see this paper:


See the doc page for the pair_style reax/c command for details of how to use it in LAMMPS.

The person who created this package is Hasan Metin Aktulga (hmaktulga at lbl.gov), while at Purdue University. Contact him directly, or Aidan Thompson at Sandia (athomps at sandia.gov), if you have questions.

**USER-SPH package**

This package implements smoothed particle hydrodynamics (SPH) in LAMMPS. Currently, the package has the following features:

* Tait, ideal gas, Lennard-Jones equation of states, full support for complete (i.e. internal-energy dependent) equations of state * plain or Monaghans XSPH integration of the equations of motion * density continuity or density summation to propagate the density field * commands to set internal energy and density of particles from the input script * output commands to access internal energy and density for dumping and thermo output

See the file doc/USER/sph/SPH_LAMMPS_userguide.pdf to get started.

There are example scripts for using this package in examples/USER/sph.

The person who created this package is Georg Ganzenmuller at the Fraunhofer-Institute for High-Speed Dynamics, Ernst Mach Institute in Germany (georg.ganzenmueller at eml.fhg.de). Contact him directly if you have questions.
5. Accelerating LAMMPS performance

This section describes various methods for improving LAMMPS performance for different classes of problems running on different kinds of machines.

5.1 Measuring performance
5.2 General strategies
5.3 Packages with optimized styles
5.4 OPT package
5.5 USER-OMP package
5.6 GPU package
5.7 USER-CUDA package
5.8 Comparison of GPU and USER-CUDA packages

5.1 Measuring performance

Before trying to make your simulation run faster, you should understand how it currently performs and where the bottlenecks are.

The best way to do this is run your system (actual number of atoms) for a modest number of timesteps (say 100, or a few 100 at most) on several different processor counts, including a single processor if possible. Do this for an equilibrium version of your system, so that the 100-step timings are representative of a much longer run. There is typically no need to run for 1000s or timesteps to get accurate timings; you can simply extrapolate from short runs.

For the set of runs, look at the timing data printed to the screen and log file at the end of each LAMMPS run. This section of the manual has an overview.

Running on one (or a few processors) should give a good estimate of the serial performance and what portions of the timestep are taking the most time. Running the same problem on a few different processor counts should give an estimate of parallel scalability. I.e. if the simulation runs 16x faster on 16 processors, its 100% parallel efficient; if it runs 8x faster on 16 processors, it's 50% efficient.

The most important data to look at in the timing info is the timing breakdown and relative percentages. For example, trying different options for speeding up the long-range solvers will have little impact if they only consume 10% of the run time. If the pairwise time is dominating, you may want to look at GPU or OMP versions of the pair style, as discussed below. Comparing how the percentages change as you increase the processor count gives you a sense of how different operations within the timestep are scaling. Note that if you are running with a Kspace solver, there is additional output on the breakdown of the Kspace time. For PPPM, this includes the fraction spent on FFTs, which can be communication intensive.

Another important detail in the timing info are the histograms of atoms counts and neighbor counts. If these vary widely across processors, you have a load-imbalance issue. This often results in inaccurate relative timing data, because processors have to wait when communication occurs for other processors to catch up. Thus the reported times for "Communication" or "Other" may be higher than they really are, due to load-imbalance. If this is an issue, you can uncomment the MPI_BARRIER() lines in src/timer.cpp, and recompile LAMMPS, to obtain synchronized timings.
5.2 General strategies

NOTE: this sub-section is still a work in progress

Here is a list of general ideas for improving simulation performance. Most of them are only applicable to certain models and certain bottlenecks in the current performance, so let the timing data you initially generate be your guide. It is hard, if not impossible, to predict how much difference these options will make, since it is a function of your problem and your machine. There is no substitute for simply trying them out.

- rRESPA
- 2-FFT PPPM
- single vs double PPPM
- partial charge PPPM
- verlet/split
- processor mapping via processors numa command
- load-balancing: balance and fix balance
- processor command for layout
- OMP when lots of cores

5.3 Packages with optimized styles

Accelerated versions of various pair_style, fixes, computes, and other commands have been added to LAMMPS, which will typically run faster than the standard non-accelerated versions, if you have the appropriate hardware on your system.

The accelerated styles have the same name as the standard styles, except that a suffix is appended. Otherwise, the syntax for the command is identical, their functionality is the same, and the numerical results it produces should also be identical, except for precision and round-off issues.

For example, all of these variants of the basic Lennard-Jones pair style exist in LAMMPS:

- pair_style lj/cut
- pair_style lj/cut/opt
- pair_style lj/cut/omp
- pair_style lj/cut/gpu
- pair_style lj/cut/cuda

Assuming you have built LAMMPS with the appropriate package, these styles can be invoked by specifying them explicitly in your input script. Or you can use the -suffix command-line switch to invoke the accelerated versions automatically, without changing your input script. The suffix command allows you to set a suffix explicitly and to turn off/on the command-line switch setting, both from within your input script.

Styles with an "opt" suffix are part of the OPT package and typically speed-up the pairwise calculations of your simulation by 5-25%.

Styles with an "omp" suffix are part of the USER-OMP package and allow a pair-style to be run in multi-threaded mode using OpenMP. This can be useful on nodes with high-core counts when using less MPI processes than cores is advantageous, e.g. when running with PPPM so that FFTs are run on fewer MPI processors or when the many MPI tasks would overload the available bandwidth for communication.

Styles with a "gpu" or "cuda" suffix are part of the GPU or USER-CUDA packages, and can be run on NVIDIA GPUs associated with your CPUs. The speed-up due to GPU usage depends on a variety of factors, as discussed.
To see what styles are currently available in each of the accelerated packages, see Section_commands 5 of the manual. A list of accelerated styles is included in the pair, fix, compute, and kspace sections.

The following sections explain:

- what hardware and software the accelerated styles require
- how to build LAMMPS with the accelerated packages in place
- what changes (if any) are needed in your input scripts
- guidelines for best performance
- speed-ups you can expect

The final section compares and contrasts the GPU and USER-CUDA packages, since they are both designed to use NVIDIA GPU hardware.

### 5.4 OPT package

The OPT package was developed by James Fischer (High Performance Technologies), David Richie, and Vincent Natoli (Stone Ridge Technologies). It contains a handful of pair styles whose compute() methods were rewritten in C++ templated form to reduce the overhead due to if tests and other conditional code.

The procedure for building LAMMPS with the OPT package is simple. It is the same as for any other package which has no additional library dependencies:

```make
make yes-opt
make machine
```

If your input script uses one of the OPT pair styles, you can run it as follows:

```bash
lmp_machine -sf opt <in.script
mpirun -np 4 lmp_machine -sf opt  <in.script
```

You should see a reduction in the "Pair time" printed out at the end of the run. On most machines and problems, this will typically be a 5 to 20% savings.

### 5.5 USER-OMP package

The USER-OMP package was developed by Axel Kohlmeyer at Temple University. It provides multi-threaded versions of most pair styles, all dihedral styles and a few fixes in LAMMPS. The package currently uses the OpenMP interface which requires using a specific compiler flag in the makefile to enable multiple threads; without this flag the corresponding pair styles will still be compiled and work, but do not support multi-threading.

**Building LAMMPS with the USER-OMP package:**

The procedure for building LAMMPS with the USER-OMP package is simple. You have to edit your machine specific makefile to add the flag to enable OpenMP support to the CCFLAGS and LINKFLAGS variables. For the GNU compilers for example this flag is called `-fopenmp`. Check your compiler documentation to find out which flag you need to add. The rest of the compilation is the same as for any other package which has no additional library dependencies:

```make
make yes-user-omp
make machine
```
Please note that this will only install accelerated versions of styles that are already installed, so you want to install this package as the last package, or else you may be missing some accelerated styles. If you plan to uninstall some package, you should first uninstall the USER-OMP package then the other package and then re-install USER-OMP, to make sure that there are no orphaned omp style files present, which would lead to compilation errors.

If your input script uses one of regular styles that are also exist as an OpenMP version in the USER-OMP package you can run it as follows:

```
env OMP_NUM_THREADS=4 lmp_serial -sf omp -in in.script
env OMP_NUM_THREADS=2 mpirun -np 2 lmp_machine -sf omp -in in.script
mpirun -x OMP_NUM_THREADS=2 -np 2 lmp_machine -sf omp -in in.script
```

The value of the environment variable OMP_NUM_THREADS determines how many threads per MPI task are launched. All three examples above use a total of 4 CPU cores. For different MPI implementations the method to pass the OMP_NUM_THREADS environment variable to all processes is different. Two different variants, one for MPICH and OpenMPI, respectively are shown above. Please check the documentation of your MPI installation for additional details. Alternatively, the value provided by OMP_NUM_THREADS can be overridden with the `package omp` command. Depending on which styles are accelerated in your input, you should see a reduction in the "Pair time" and/or "Bond time" and "Loop time" printed out at the end of the run. The optimal ratio of MPI to OpenMP can vary a lot and should always be confirmed through some benchmark runs for the current system and on the current machine.

**Restrictions:**

None of the pair styles in the USER-OMP package support the "inner", "middle", "outer" options for r-RESPA integration, only the "pair" option is supported.

**Parallel efficiency and performance tips:**

In most simple cases the MPI parallelization in LAMMPS is more efficient than multi-threading implemented in the USER-OMP package. Also the parallel efficiency varies between individual styles. On the other hand, in many cases you still want to use the omp version - even when compiling or running without OpenMP support - since they all contain optimizations similar to those in the OPT package, which can result in serial speedup.

Using multi-threading is most effective under the following circumstances:

- Individual compute nodes have a significant number of CPU cores but the CPU itself has limited memory bandwidth, e.g. Intel Xeon 53xx (Clovertown) and 54xx (Harpertown) quad core processors. Running one MPI task per CPU core will result in significant performance degradation, so that running with 4 or even only 2 MPI tasks per nodes is faster. Running in hybrid MPI+OpenMP mode will reduce the inter-node communication bandwidth contention in the same way, but offers and additional speedup from utilizing the otherwise idle CPU cores.
- The interconnect used for MPI communication is not able to provide sufficient bandwidth for a large number of MPI tasks per node. This applies for example to running over gigabit ethernet or on Cray XT4 or XT5 series supercomputers. Same as in the aforementioned case this effect worsens with using an increasing number of nodes.
- The input is a system that has an inhomogeneous particle density which cannot be mapped well to the domain decomposition scheme that LAMMPS employs. While this can be to some degree alleviated through using the `processors` keyword, multi-threading provides a parallelism that parallelizes over the number of particles not their distribution in space.
- Finally, multi-threaded styles can improve performance when running LAMMPS in "capability mode", i.e. near the point where the MPI parallelism scales out. This can happen in particular when using as
kspace style for long-range electrostatics. Here the scaling of the kspace style is the performance limiting factor and using multi-threaded styles allows to operate the kspace style at the limit of scaling and then increase performance parallelizing the real space calculations with hybrid MPI+OpenMP. Sometimes additional speedup can be achieved by increasing the real-space coulomb cutoff and thus reducing the work in the kspace part.

The best parallel efficiency from *omp* styles is typically achieved when there is at least one MPI task per physical processor, i.e. socket or die.

Using threads on hyper-threading enabled cores is usually counterproductive, as the cost in additional memory bandwidth requirements is not offset by the gain in CPU utilization through hyper-threading.

A description of the multi-threading strategy and some performance examples are presented here.

## 5.6 GPU package

The GPU package was developed by Mike Brown at ORNL. It provides GPU versions of several pair styles and for long-range Coulombics via the PPPM command. It has the following features:

- The package is designed to exploit common GPU hardware configurations where one or more GPUs are coupled with many cores of a multi-core CPUs, e.g. within a node of a parallel machine.
- Atom-based data (e.g. coordinates, forces) moves back-and-forth between the CPU(s) and GPU every timestep.
- Neighbor lists can be constructed on the CPU or on the GPU.
- The charge assignment and force interpolation portions of PPPM can be run on the GPU. The FFT portion, which requires MPI communication between processors, runs on the CPU.
- Asynchronous force computations can be performed simultaneously on the CPU(s) and GPU.
- LAMMPS-specific code is in the GPU package. It makes calls to a generic GPU library in the lib/gpu directory. This library provides NVIDIA support as well as more general OpenCL support, so that the same functionality can eventually be supported on a variety of GPU hardware.

NOTE: discuss 3 precisions if change, also have to re-link with LAMMPS always use newton off expt with differing numbers of CPUs vs GPU - can't tell what is fastest give command line switches in examples

### Hardware and software requirements:

To use this package, you currently need to have specific NVIDIA hardware and install specific NVIDIA CUDA software on your system:

- Check if you have an NVIDIA card: `cat /proc/driver/nvidia/cards/0`
- Install a driver and toolkit appropriate for your system (SDK is not necessary)
- Follow the instructions in `lammps/lib/gpu/README` to build the library (see below)
- Run `lammps/lib/gpu/nvc_get_devices` to list supported devices and properties

### Building LAMMPS with the GPU package:

As with other packages that include a separately compiled library, you need to first build the GPU library, before building LAMMPS itself. General instructions for doing this are in this section of the manual. For this package, do the following, using a Makefile in lib/gpu appropriate for your system:

```
cd lammps/lib/gpu
make -f Makefile.linux
```
If you are successful, you will produce the file lib/libgpu.a.

Now you are ready to build LAMMPS with the GPU package installed:

cd lammps/src
make yes-gpu
make machine

Note that the lo-level Makefile (e.g. src/MAKE/Makefile.linux) has these settings: gpu_SYSINC, gpu_SYSLIB, gpu_SYSPATH. These need to be set appropriately to include the paths and settings for the CUDA system software on your machine. See src/MAKE/Makefile.g++ for an example.

**GPU configuration**

When using GPUs, you are restricted to one physical GPU per LAMMPS process, which is an MPI process running on a single core or processor. Multiple MPI processes (CPU cores) can share a single GPU, and in many cases it will be more efficient to run this way.

**Input script requirements:**

Additional input script requirements to run pair or PPPM styles with a `gpu` suffix are as follows:

- To invoke specific styles from the GPU package, you can either append "gpu" to the style name (e.g. `pair_style lj/cut/gpu`), or use the `-suffix` command-line switch, or use the `suffix` command.
- The `newton pair` setting must be `off`.
- The `package gpu` command must be used near the beginning of your script to control the GPU selection and initialization settings. It also has an option to enable asynchronous splitting of force computations between the CPUs and GPUs.

As an example, if you have two GPUs per node and 8 CPU cores per node, and would like to run on 4 nodes (32 cores) with dynamic balancing of force calculation across CPU and GPU cores, you could specify

```
package gpu force/neigh 0 1 -1
```

In this case, all CPU cores and GPU devices on the nodes would be utilized. Each GPU device would be shared by 4 CPU cores. The CPU cores would perform force calculations for some fraction of the particles at the same time the GPUs performed force calculation for the other particles.

**Timing output:**

As described by the `package gpu` command, GPU accelerated pair styles can perform computations asynchronously with CPU computations. The "Pair" time reported by LAMMPS will be the maximum of the time required to complete the CPU pair style computations and the time required to complete the GPU pair style computations. Any time spent for GPU-enabled pair styles for computations that run simultaneously with bond, angle, dihedral, improper, and long-range calculations will not be included in the "Pair" time.

When the `mode` setting for the package gpu command is force/neigh, the time for neighbor list calculations on the GPU will be added into the "Pair" time, not the "Neigh" time. An additional breakdown of the times required for various tasks on the GPU (data copy, neighbor calculations, force computations, etc) are output only with the LAMMPS screen output (not in the log file) at the end of each run. These timings represent total time spent on the GPU for each routine, regardless of asynchronous CPU calculations.
Performance tips:

Generally speaking, for best performance, you should use multiple CPUs per GPU, as provided my most multi-core CPU/GPU configurations.

Because of the large number of cores within each GPU device, it may be more efficient to run on fewer processes per GPU when the number of particles per MPI process is small (100’s of particles); this can be necessary to keep the GPU cores busy.

See the lammps/lib/gpu/README file for instructions on how to build the GPU library for single, mixed, or double precision. The latter requires that your GPU card support double precision.

5.7 USER-CUDA package

The USER-CUDA package was developed by Christian Trott at U Technology Ilmenau in Germany. It provides NVIDIA GPU versions of many pair styles, many fixes, a few computes, and for long-range Coulombics via the PPPM command. It has the following features:

- The package is designed to allow an entire LAMMPS calculation, for many timesteps, to run entirely on the GPU (except for inter-processor MPI communication), so that atom-based data (e.g. coordinates, forces) do not have to move back-and-forth between the CPU and GPU.
- The speed-up advantage of this approach is typically better when the number of atoms per GPU is large
- Data will stay on the GPU until a timestep where a non-GPU-ized fix or compute is invoked. Whenever a non-GPU operation occurs (fix, compute, output), data automatically moves back to the CPU as needed. This may incur a performance penalty, but should otherwise work transparently.
- Neighbor lists for GPU-ized pair styles are constructed on the GPU.
- The package only supports use of a single CPU (core) with each GPU.

Hardware and software requirements:

To use this package, you need to have specific NVIDIA hardware and install specific NVIDIA CUDA software on your system.

Your NVIDIA GPU needs to support Compute Capability 1.3. This list may help you to find out the Compute Capability of your card:

http://en.wikipedia.org/wiki/Comparison_of_Nvidia_graphics_processing_units

Install the Nvidia Cuda Toolkit in version 3.2 or higher and the corresponding GPU drivers. The Nvidia Cuda SDK is not required for LAMMPSCUDA but we recommend it be installed. You can then make sure that its sample projects can be compiled without problems.

Building LAMMPS with the USER-CUDA package:

As with other packages that include a separately compiled library, you need to first build the USER-CUDA library, before building LAMMPS itself. General instructions for doing this are in this section of the manual. For this package, do the following, using settings in the lib/cuda Makefiles appropriate for your system:

- Go to the lammps/lib/cuda directory
- If your CUDA toolkit is not installed in the default system directory /usr/local/cuda edit the file lib/cuda/Makefile.common accordingly.
• Type "make OPTIONS", where OPTIONS are one or more of the following options. The settings will be written to the lib/cuda/Makefile.defaults and used in the next step.

    precision=N to set the precision level
    N = 1 for single precision (default)
    N = 2 for double precision
    N = 3 for positions in double precision
    N = 4 for positions and velocities in double precision
    arch=M to set GPU compute capability
    M = 20 for CC2.0 (GF100/110, e.g. C2050,GTX580,GTX470) (default)
    M = 21 for CC2.1 (GF104/114, e.g. GTX560, GTX460, GTX450)
    M = 13 for CC1.3 (GF200, e.g. C1060, GTX285)
    prec_timer=0/1 to use hi-precision timers
    0 = do not use them (default)
    1 = use these timers
    this is usually only useful for Mac machines
    dbg=0/1 to activate debug mode
    0 = no debug mode (default)
    1 = yes debug mode
    this is only useful for developers
    cufft=1 to determine usage of CUDA FFT library
    0 = no CUFFT support (default)
    in the future other CUDA-enabled FFT libraries might be supported

• Type "make" to build the library. If you are successful, you will produce the file lib/libcuda.a.

Now you are ready to build LAMMPS with the USER-CUDA package installed:

    cd lammps/src
    make yes-user-cuda
    make machine

Note that the LAMMPS build references the lib/cuda/Makefile.common file to extract setting specific CUDA settings. So it is important that you have first built the cuda library (in lib/cuda) using settings appropriate to your system.

Input script requirements:

Additional input script requirements to run styles with a cuda suffix are as follows:

• To invoke specific styles from the USER-CUDA package, you can either append "cuda" to the style name (e.g. pair_style lj/cut/cuda), or use the -suffix command-line switch, or use the suffix command. One exception is that the kspace_style pppm/cuda command has to be requested explicitly.
• To use the USER-CUDA package with its default settings, no additional command is needed in your input script. This is because when LAMMPS starts up, it detects if it has been built with the USER-CUDA package. See the -cuda command-line switch for more details.
• To change settings for the USER-CUDA package at run-time, the package cuda command can be used near the beginning of your input script. See the package command doc page for details.

Performance tips:

The USER-CUDA package offers more speed-up relative to CPU performance when the number of atoms per GPU is large, e.g. on the order of tens or hundreds of 1000s.

As noted above, this package will continue to run a simulation entirely on the GPU(s) (except for inter-processor MPI communication), for multiple timesteps, until a CPU calculation is required, either by a fix or compute that is non-GPU-ized, or until output is performed (thermo or dump snapshot or restart file). The less often this occurs, the faster your simulation will run.
5.8 Comparison of GPU and USER-CUDA packages

Both the GPU and USER-CUDA packages accelerate a LAMMPS calculation using NVIDIA hardware, but they do it in different ways.

As a consequence, for a particular simulation on specific hardware, one package may be faster than the other. We give guidelines below, but the best way to determine which package is faster for your input script is to try both of them on your machine. See the benchmarking section below for examples where this has been done.

Guidelines for using each package optimally:

- The GPU package allows you to assign multiple CPUs (cores) to a single GPU (a common configuration for "hybrid" nodes that contain multicore CPU(s) and GPU(s)) and works effectively in this mode. The USER-CUDA package does not allow this; you can only use one CPU per GPU.
- The GPU package moves per-atom data (coordinates, forces) back-and-forth between the CPU and GPU every timestep. The USER-CUDA package only does this on timesteps when a CPU calculation is required (e.g. to invoke a fix or compute that is non-GPU-ized). Hence, if you can formulate your input script to only use GPU-ized fixes and computes, and avoid doing I/O too often (thermo output, dump file snapshots, restart files), then the data transfer cost of the USER-CUDA package can be very low, causing it to run faster than the GPU package.
- The GPU package is often faster than the USER-CUDA package, if the number of atoms per GPU is "small". The crossover point, in terms of atoms/GPU at which the USER-CUDA package becomes faster depends strongly on the pair style. For example, for a simple Lennard Jones system the crossover (in single precision) is often about 50K-100K atoms per GPU. When performing double precision calculations the crossover point can be significantly smaller.
- Both packages compute bonded interactions (bonds, angles, etc) on the CPU. This means a model with bonds will force the USER-CUDA package to transfer per-atom data back-and-forth between the CPU and GPU every timestep. If the GPU package is running with several MPI processes assigned to one GPU, the cost of computing the bonded interactions is spread across more CPUs and hence the GPU package can run faster.
- When using the GPU package with multiple CPUs assigned to one GPU, its performance depends to some extent on high bandwidth between the CPUs and the GPU. Hence its performance is affected if full 16 PCIe lanes are not available for each GPU. In HPC environments this can be the case if S2050/70 servers are used, where two devices generally share one PCIe 2.0 16x slot. Also many multi-GPU mainboards do not provide full 16 lanes to each of the PCIe 2.0 16x slots.

Differences between the two packages:

- The GPU package accelerates only pair force, neighbor list, and PPPM calculations. The USER-CUDA package currently supports a wider range of pair styles and can also accelerate many fix styles and some compute styles, as well as neighbor list and PPPM calculations.
- The USER-CUDA package does not support acceleration for minimization.
- The USER-CUDA package does not support hybrid pair styles.
- The USER-CUDA package can order atoms in the neighbor list differently from run to run resulting in a different order for force accumulation.
- The USER-CUDA package has a limit on the number of atom types that can be used in a simulation.
- The GPU package requires neighbor lists to be built on the CPU when using exclusion lists or a triclinic simulation box.
- The GPU package uses more GPU memory than the USER-CUDA package. This is generally not a problem since typical runs are computation-limited rather than memory-limited.
Examples:

The LAMMPS distribution has two directories with sample input scripts for the GPU and USER-CUDA packages.

- `lammps/examples/gpu` = GPU package files
- `lammps/examples/USER/cuda` = USER-CUDA package files

These contain input scripts for identical systems, so they can be used to benchmark the performance of both packages on your system.
6. How-to discussions

This section describes how to perform common tasks using LAMMPS.

6.1 Restarting a simulation
6.2 2d simulations
6.3 CHARMM, AMBER, and DREIDING force fields
6.4 Running multiple simulations from one input script
6.5 Multi-replica simulations
6.6 Granular models
6.7 TIP3P water model
6.8 TIP4P water model
6.9 SPC water model
6.10 Coupling LAMMPS to other codes
6.11 Visualizing LAMMPS snapshots
6.12 Triclinic (non-orthogonal) simulation boxes
6.13 NEMD simulations
6.14 Extended spherical and aspherical particles
6.15 Output from LAMMPS (thermo, dumps, computes, fixes, variables)
6.16 Thermostating, barostatting and computing temperature
6.17 Walls
6.18 Elastic constants
6.19 Library interface to LAMMPS
6.20 Calculating thermal conductivity
6.21 Calculating viscosity

The example input scripts included in the LAMMPS distribution and highlighted in Section_example also show how to setup and run various kinds of simulations.

6.1 Restarting a simulation

There are 3 ways to continue a long LAMMPS simulation. Multiple run commands can be used in the same input script. Each run will continue from where the previous run left off. Or binary restart files can be saved to disk using the restart command. At a later time, these binary files can be read via a read_restart command in a new script. Or they can be converted to text data files and read by a read_data command in a new script. This section discusses the restart2data tool that is used to perform the conversion.

Here we give examples of 2 scripts that read either a binary restart file or a converted data file and then issue a new run command to continue where the previous run left off. They illustrate what settings must be made in the new script. Details are discussed in the documentation for the read_restart and read_data commands.

Look at the in.chain input script provided in the bench directory of the LAMMPS distribution to see the original script that these 2 scripts are based on. If that script had the line

```
restart         50 tmp.restart
```

added to it, it would produce 2 binary restart files (tmp.restart.50 and tmp.restart.100) as it ran.
This script could be used to read the 1st restart file and re-run the last 50 timesteps:

```plaintext
read_restart    tmp.restart.50
neighbor        0.4 bin
neigh_modify    every 1 delay 1
fix             1 all nve
fix             2 all langevin 1.0 1.0 10.0 904297

run             50
```

Note that the following commands do not need to be repeated because their settings are included in the restart file: `units, atom_style, special_bonds, pair_style, bond_style`. However these commands do need to be used, since their settings are not in the restart file: `neighbor, fix, timestep`.

If you actually use this script to perform a restarted run, you will notice that the thermodynamic data match at step 50 (if you also put a "thermo 50" command in the original script), but do not match at step 100. This is because the `fix langevin` command uses random numbers in a way that does not allow for perfect restarts.

As an alternate approach, the restart file could be converted to a data file using this tool:

```plaintext
restart2data tmp.restart.50 tmp.restart.data
```

Then, this script could be used to re-run the last 50 steps:

```plaintext
units           lj
atom_style      bond
pair_style      lj/cut 1.12
pair_modify     shift yes
bond_style      fene
special_bonds   0.0 1.0 1.0

read_data       tmp.restart.data

neighbor        0.4 bin
neigh_modify    every 1 delay 1
fix             1 all nve
fix             2 all langevin 1.0 1.0 10.0 904297

run             50
```

Note that nearly all the settings specified in the original `in.chain` script must be repeated, except the `pair_coeff` and `bond_coeff` commands since the new data file lists the force field coefficients. Also, the `reset_timestep` command is used to tell LAMMPS the current timestep. This value is stored in restart files, but not in data files.
6.2 2d simulations

Use the `dimension` command to specify a 2d simulation.

Make the simulation box periodic in z via the `boundary` command. This is the default.

If using the `create box` command to define a simulation box, set the z dimensions narrow, but finite, so that the `create_atoms` command will tile the 3d simulation box with a single z plane of atoms - e.g.

```plaintext
create box 1 -10 10 -10 10 -0.25 0.25
```

If using the `read data` command to read in a file of atom coordinates, set the "zlo zhi" values to be finite but narrow, similar to the `create_box` command settings just described. For each atom in the file, assign a z coordinate so it falls inside the z-boundaries of the box - e.g. 0.0.

Use the `fix enforce2d` command as the last defined fix to insure that the z-components of velocities and forces are zeroed out every timestep. The reason to make it the last fix is so that any forces induced by other fixes will be zeroed out.

Many of the example input scripts included in the LAMMPS distribution are for 2d models.

IMPORTANT NOTE: Some models in LAMMPS treat particles as extended spheres, as opposed to point particles. In 2d, the particles will still be spheres, not disks, meaning their moment of inertia will be the same as in 3d.

6.3 CHARMM, AMBER, and DREIDING force fields

A force field has 2 parts: the formulas that define it and the coefficients used for a particular system. Here we only discuss formulas implemented in LAMMPS that correspond to formulas commonly used in the CHARMM, AMBER, and DREIDING force fields. Setting coefficients is done in the input data file via the `read_data` command or in the input script with commands like `pair_coeff` or `bond_coeff`. See Section_tools for additional tools that can use CHARMM or AMBER to assign force field coefficients and convert their output into LAMMPS input.

See (MacKerell) for a description of the CHARMM force field. See (Cornell) for a description of the AMBER force field.

These style choices compute force field formulas that are consistent with common options in CHARMM or AMBER. See each command's documentation for the formula it computes.

- `bond_style` harmonic
- `angle_style` charmm
- `dihedral_style` charmm
- `pair_style` lj/charmm/coul/charmm
- `pair_style` lj/charmm/coul/charmm/implicit
- `pair_style` lj/charmm/coul/long
- `special_bonds` charmm
- `special_bonds` amber

DREIDING is a generic force field developed by the Goddard group at Caltech and is useful for predicting
structures and dynamics of organic, biological and main-group inorganic molecules. The philosophy in
DREIDING is to use general force constants and geometry parameters based on simple hybridization
considerations, rather than individual force constants and geometric parameters that depend on the particular
combinations of atoms involved in the bond, angle, or torsion terms. DREIDING has an explicit hydrogen bond
term to describe interactions involving a hydrogen atom on very electronegative atoms (N, O, F).

See (Mayo) for a description of the DREIDING force field

These style choices compute force field formulas that are consistent with the DREIDING force field. See each
command's documentation for the formula it computes.

- bond_style harmonic
- bond_style morse
- angle_style harmonic
- angle_style cosine
- angle_style cosine/periodic
- dihedral_style charmm
- improper_style umbrella
- pair_style buck
- pair_style buck/coul/cut
- pair_style buck/coul/long
- pair_style lj/cut
- pair_style lj/cut/coul/cut
- pair_style lj/cut/coul/long
- pair_style hbond/dreiding/lj
- pair_style hbond/dreiding/morse
- special_bonds dreiding

6.4 Running multiple simulations from one input script

This can be done in several ways. See the documentation for individual commands for more details on how these
examples work.

If "multiple simulations" means continue a previous simulation for more timesteps, then you simply use the run
command multiple times. For example, this script

```
units lj
atom_style atomic
read_data data.lj
run 10000
run 10000
run 10000
run 10000
run 10000
```

would run 5 successive simulations of the same system for a total of 50,000 timesteps.
If you wish to run totally different simulations, one after the other, the clear command can be used in between them to re-initialize LAMMPS. For example, this script

```
units lj
atom_style atomic
read_data data.lj
run 10000
clear
units lj
atom_style atomic
read_data data.lj.new
run 10000
```

would run 2 independent simulations, one after the other.

For large numbers of independent simulations, you can use variables and the next and jump commands to loop over the same input script multiple times with different settings. For example, this script, named in.polymer

```
variable d index run1 run2 run3 run4 run5 run6 run7 run8
shell cd $d
read_data data.polymer
run 10000
shell cd ..
clear
next d
jump in.polymer
```

would run 8 simulations in different directories, using a data.polymer file in each directory. The same concept could be used to run the same system at 8 different temperatures, using a temperature variable and storing the output in different log and dump files, for example

```
variable a loop 8
variable t index 0.8 0.85 0.9 0.95 1.0 1.05 1.1 1.15
log log.$a
read data.polymer
velocity all create $t 352839
fix 1 all nvt $t $t 100.0
dump 1 all atom 1000 dump.$a
run 100000
next t
next a
jump in.polymer
```

All of the above examples work whether you are running on 1 or multiple processors, but assumed you are running LAMMPS on a single partition of processors. LAMMPS can be run on multiple partitions via the "-partition" command-line switch as described in this section of the manual.

In the last 2 examples, if LAMMPS were run on 3 partitions, the same scripts could be used if the "index" and "loop" variables were replaced with universe-style variables, as described in the variable command. Also, the "next t" and "next a" commands would need to be replaced with a single "next a t" command. With these modifications, the 8 simulations of each script would run on the 3 partitions one after the other until all were finished. Initially, 3 simulations would be started simultaneously, one on each partition. When one finished, that partition would then start the 4th simulation, and so forth, until all 8 were completed.
6.5 Multi-replica simulations

Several commands in LAMMPS run multi-replica simulations, meaning that multiple instances (replicas) of your simulation are run simultaneously, with small amounts of data exchanged between replicas periodically.

These are the relevant commands:

- **neb** for nudged elastic band calculations
- **prd** for parallel replica dynamics
- **tad** for temperature accelerated dynamics
- **temper** for parallel tempering

NEB is a method for finding transition states and barrier energies. PRD and TAD are methods for performing accelerated dynamics to find and perform infrequent events. Parallel tempering or replica exchange runs different replicas at a series of temperature to facilitate rare-event sampling.

These command can only be used if LAMMPS was built with the "replica" package. See the Making LAMMPS section for more info on packages.

In all these cases, you must run with one or more processors per replica. The processors assigned to each replica are determined at run-time by using the **-partition command-line switch** to launch LAMMPS on multiple partitions, which in this context are the same as replicas. E.g. these commands:

```bash
mpirun -np 16 lmp_linux -partition 8x2 -in in.temper
mpirun -np 8 lmp_linux -partition 8x1 -in in.neb
```

would each run 8 replicas, on either 16 or 8 processors. Note the use of the **-in command-line switch** to specify the input script which is required when running in multi-replica mode.

Also note that with MPI installed on a machine (e.g. your desktop), you can run on more (virtual) processors than you have physical processors. Thus the above commands could be run on a single-processor (or few-processor) desktop so that you can run a multi-replica simulation on more replicas than you have physical processors.

6.6 Granular models

Granular system are composed of spherical particles with a diameter, as opposed to point particles. This means they have an angular velocity and torque can be imparted to them to cause them to rotate.

To run a simulation of a granular model, you will want to use the following commands:

- **atom_style** sphere
- **fix nve/sphere**
- **fix gravity**

This compute

- **compute erotate/sphere**

calculates rotational kinetic energy which can be **output with thermodynamic info**.

Use one of these 3 pair potentials, which compute forces and torques between interacting pairs of particles:
These commands implement fix options specific to granular systems:

- fix freeze
- fix pour
- fix viscous
- fix wall/gran

The fix style *freeze* zeroes both the force and torque of frozen atoms, and should be used for granular systems instead of the fix style *setforce*.

For computational efficiency, you can eliminate needless pairwise computations between frozen atoms by using this command:

```
neigh_modify exclude
```

### 6.7 TIP3P water model

The TIP3P water model as implemented in CHARMM (MacKerell) specifies a 3-site rigid water molecule with charges and Lennard-Jones parameters assigned to each of the 3 atoms. In LAMMPS the fix shake command can be used to hold the two O-H bonds and the H-O-H angle rigid. A bond style of *harmonic* and an angle style of *harmonic* or *charmm* should also be used.

These are the additional parameters (in real units) to set for O and H atoms and the water molecule to run a rigid TIP3P-CHARMM model with a cutoff. The K values can be used if a flexible TIP3P model (without fix shake) is desired. If the LJ epsilon and sigma for HH and OH are set to 0.0, it corresponds to the original 1983 TIP3P model (Jorgensen).

```
O mass = 15.9994
H mass = 1.008
O charge = -0.834
H charge = 0.417
LJ epsilon of OO = 0.1521
LJ sigma of OO = 3.1507
LJ epsilon of HH = 0.0460
LJ sigma of HH = 0.4000
LJ epsilon of OH = 0.0836
LJ sigma of OH = 1.7753
K of OH bond = 450
r0 of OH bond = 0.9572
K of HOH angle = 55
theta of HOH angle = 104.52
```
These are the parameters to use for TIP3P with a long-range Coulombic solver (Ewald or PPPM in LAMMPS), see (Price) for details:

O mass = 15.9994
H mass = 1.008

O charge = -0.830
H charge = 0.415

LJ epsilon of OO = 0.102
LJ sigma of OO = 3.188
LJ epsilon, sigma of OH, HH = 0.0

K of OH bond = 450
r0 of OH bond = 0.9572

K of HOH angle = 55
theta of HOH angle = 104.52

Wikipedia also has a nice article on water models.

6.8 TIP4P water model

The four-point TIP4P rigid water model extends the traditional three-point TIP3P model by adding an additional site, usually massless, where the charge associated with the oxygen atom is placed. This site M is located at a fixed distance away from the oxygen along the bisector of the HOH bond angle. A bond style of harmonic and an angle style of harmonic or charmm should also be used.

A TIP4P model is run with LAMMPS using two commands:

- pair_style lj/cut/coul/long/tip4p
- kspace_style pppm/tip4p

Note that only a TIP4P model with long-range Coulombics is currently implemented. A cutoff version may be added in the future. for both models, the bond lengths and bond angles should be held fixed using the fix shake command.

These are the additional parameters (in real units) to set for O and H atoms and the water molecule to run a rigid TIP4P model with a cutoff (Jorgensen). Note that the OM distance is specified in the pair_style command, not as part of the pair coefficients.

O mass = 15.9994
H mass = 1.008

O charge = -1.040
H charge = 0.520

r0 of OH bond = 0.9572
theta of HOH angle = 104.52

OM distance = 0.15
LJ epsilon of O-O = 0.1550
LJ sigma of O-O = 3.1536
LJ epsilon, sigma of OH, HH = 0.0

These are the parameters to use for TIP4P with a long-range Coulombic solver (Ewald or PPPM in LAMMPS):

O mass = 15.9994
H mass = 1.008

O charge = -1.0484
H charge = 0.5242

r0 of OH bond = 0.9572
theta of HOH angle = 104.52

OM distance = 0.1250

LJ epsilon of O-O = 0.16275
LJ sigma of O-O = 3.16435
LJ epsilon, sigma of OH, HH = 0.0

Note that the when using the TIP4P pair style, the neighobr list cutoff for Coulomb interactions is effectively extended by a distance 2 * (OM distance), to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff >= Coulomb cutoff + 2*(OM distance), to shrink the size of the neighbor list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model. The OM distance and the LJ and Coulombic cutoffs are set in the pair_style lj/cut/coul/long/tip4p command.

Wikipedia also has a nice article on water models.

---

### 6.9 SPC water model

The SPC water model specifies a 3-site rigid water molecule with charges and Lennard-Jones parameters assigned to each of the 3 atoms. In LAMMPS the fix shake command can be used to hold the two O-H bonds and the H-O-H angle rigid. A bond style of harmonic and an angle style of harmonic or charmm should also be used.

These are the additional parameters (in real units) to set for O and H atoms and the water molecule to run a rigid SPC model.

O mass = 15.9994
H mass = 1.008

O charge = -0.820
H charge = 0.410

LJ epsilon of OO = 0.1553
LJ sigma of OO = 3.166
LJ epsilon, sigma of OH, HH = 0.0

r0 of OH bond = 1.0
theta of HOH angle = 109.47
Note that as originally proposed, the SPC model was run with a 9 Angstrom cutoff for both LJ and Coulombic terms. It can also be used with long-range Coulombs (Ewald or PPPM in LAMMPS), without changing any of the parameters above, though it becomes a different model in that mode of usage.

The SPC/E (extended) water model is the same, except the partial charge assignments change:

O charge = -0.8476  
H charge = 0.4238

See the (Berendsen) reference for more details on both the SPC and SPC/E models.

Wikipedia also has a nice article on water models.

6.10 Coupling LAMMPS to other codes

LAMMPS is designed to allow it to be coupled to other codes. For example, a quantum mechanics code might compute forces on a subset of atoms and pass those forces to LAMMPS. Or a continuum finite element (FE) simulation might use atom positions as boundary conditions on FE nodal points, compute a FE solution, and return interpolated forces on MD atoms.

LAMMPS can be coupled to other codes in at least 3 ways. Each has advantages and disadvantages, which you'll have to think about in the context of your application.

(1) Define a new fix command that calls the other code. In this scenario, LAMMPS is the driver code. During its timestepping, the fix is invoked, and can make library calls to the other code, which has been linked to LAMMPS as a library. This is the way the POEMS package that performs constrained rigid-body motion on groups of atoms is hooked to LAMMPS. See the fix_poems command for more details. See this section of the documentation for info on how to add a new fix to LAMMPS.

(2) Define a new LAMMPS command that calls the other code. This is conceptually similar to method (1), but in this case LAMMPS and the other code are on a more equal footing. Note that now the other code is not called during the timestepping of a LAMMPS run, but between runs. The LAMMPS input script can be used to alternate LAMMPS runs with calls to the other code, invoked via the new command. The run command facilitates this with its every option, which makes it easy to run a few steps, invoke the command, run a few steps, invoke the command, etc.

In this scenario, the other code can be called as a library, as in (1), or it could be a stand-alone code, invoked by a system() call made by the command (assuming your parallel machine allows one or more processors to start up another program). In the latter case the stand-alone code could communicate with LAMMPS thru files that the command writes and reads.

See Section_modify of the documentation for how to add a new command to LAMMPS.

(3) Use LAMMPS as a library called by another code. In this case the other code is the driver and calls LAMMPS as needed. Or a wrapper code could link and call both LAMMPS and another code as libraries. Again, the run command has options that allow it to be invoked with minimal overhead (no setup or clean-up) if you wish to do multiple short runs, driven by another program.

Examples of driver codes that call LAMMPS as a library are included in the examples/COUPLE directory of the LAMMPS distribution; see examples/COUPLE/README for more details:
• simple: simple driver programs in C++ and C which invoke LAMMPS as a library
• lammps_quest: coupling of LAMMPS and Quest, to run classical MD with quantum forces calculated by a density functional code
• lammps_spparks: coupling of LAMMPS and SPPARKS, to couple a kinetic Monte Carlo model for grain growth using MD to calculate strain induced across grain boundaries

This section of the documentation describes how to build LAMMPS as a library. Once this is done, you can interface with LAMMPS either via C++, C, Fortran, or Python (or any other language that supports a vanilla C-like interface). For example, from C++ you could create one (or more) "instances" of LAMMPS, pass it an input script to process, or execute individual commands, all by invoking the correct class methods in LAMMPS. From C or Fortran you can make function calls to do the same things. See Section_python of the manual for a description of the Python wrapper provided with LAMMPS that operates through the LAMMPS library interface.

The files src/library.cpp and library.h contain the C-style interface to LAMMPS. See Section_howto 19 of the manual for a description of the interface and how to extend it for your needs.

Note that the lammps_open() function that creates an instance of LAMMPS takes an MPI communicator as an argument. This means that instance of LAMMPS will run on the set of processors in the communicator. Thus the calling code can run LAMMPS on all or a subset of processors. For example, a wrapper script might decide to alternate between LAMMPS and another code, allowing them both to run on all the processors. Or it might allocate half the processors to LAMMPS and half to the other code and run both codes simultaneously before syncing them up periodically. Or it might instantiate multiple instances of LAMMPS to perform different calculations.

6.11 Visualizing LAMMPS snapshots

LAMMPS itself does not do visualization, but snapshots from LAMMPS simulations can be visualized (and analyzed) in a variety of ways.

LAMMPS snapshots are created by the dump command which can create files in several formats. The native LAMMPS dump format is a text file (see "dump atom" or "dump custom") which can be visualized by the xmovie program, included with the LAMMPS package. This produces simple, fast 2d projections of 3d systems, and can be useful for rapid debugging of simulation geometry and atom trajectories.

Several programs included with LAMMPS as auxiliary tools can convert native LAMMPS dump files to other formats. See the Section_tools doc page for details. The first is the ch2lmp tool, which contains a lammps2pdb Perl script which converts LAMMPS dump files into PDB files. The second is the lmp2arc tool which converts LAMMPS dump files into Accelrys' Insight MD program files. The third is the lmp2cfg tool which converts LAMMPS dump files into CFG files which can be read into the AtomEye visualizer.

A Python-based toolkit distributed by our group can read native LAMMPS dump files, including custom dump files with additional columns of user-specified atom information, and convert them to various formats or pipe them into visualization software directly. See the Pizza.py WWW site for details. Specifically, Pizza.py can convert LAMMPS dump files into PDB, XYZ, Ensight, and VTK formats. Pizza.py can pipe LAMMPS dump files directly into the Raster3d and RasMol visualization programs. Pizza.py has tools that do interactive 3d OpenGL visualization and one that creates SVG images of dump file snapshots.

LAMMPS can create XYZ files directly (via "dump xyz") which is a simple text-based file format used by many visualization programs including VMD.
LAMMPS can create DCD files directly (via "dump dcd") which can be read by VMD in conjunction with a CHARMM PSF file. Using this form of output avoids the need to convert LAMMPS snapshots to PDB files. See the dump command for more information on DCD files.

LAMMPS can create XTC files directly (via "dump xtc") which is GROMACS file format which can also be read by VMD for visualization. See the dump command for more information on XTC files.

### 6.12 Triclinic (non-orthogonal) simulation boxes

By default, LAMMPS uses an orthogonal simulation box to encompass the particles. The boundary command sets the boundary conditions of the box (periodic, non-periodic, etc). The orthogonal box has its "origin" at \((x_{lo}, y_{lo}, z_{lo})\) and is defined by 3 edge vectors starting from the origin given by \( \mathbf{a} = (x_{hi} - x_{lo}, 0, 0); \mathbf{b} = (0, y_{hi} - y_{lo}, 0); \mathbf{c} = (0, 0, z_{hi} - z_{lo}) \). The 6 parameters \((x_{lo}, x_{hi}, y_{lo}, y_{hi}, z_{lo}, z_{hi})\) are defined at the time the simulation box is created, e.g. by the create_box or read_data or read_restart commands. Additionally, LAMMPS defines box size parameters \(l_x, l_y, l_z\) where \(l_x = x_{hi} - x_{lo}\), and similarly in the y and z dimensions. The 6 parameters, as well as \(l_x, l_y, l_z\), can be output via the thermo_style custom command.

LAMMPS also allows simulations to be performed in triclinic (non-orthogonal) simulation boxes shaped as a parallelepiped with triclinic symmetry. The parallelepiped has its "origin" at \((x_{lo}, y_{lo}, z_{lo})\) and is defined by 3 edge vectors starting from the origin given by \( \mathbf{a} = (x_{hi} - x_{lo}, 0, 0); \mathbf{b} = (xy, y_{hi} - y_{lo}, 0); \mathbf{c} = (xz, yz, z_{hi} - z_{lo}) \). \(xy, xz, yz\) can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped. In LAMMPS the triclinic simulation box edge vectors \(\mathbf{a}, \mathbf{b}, \mathbf{c}\) cannot be arbitrary vectors. As indicated, \(\mathbf{a}\) must lie on the positive x axis, \(\mathbf{b}\) must lie in the xy plane, with strictly positive y component. \(\mathbf{c}\) may have any orientation with strictly positive z component. The requirement that \(\mathbf{a}, \mathbf{b}, \mathbf{c}\) have strictly positive x, y, and z components, respectively, ensures that \(\mathbf{a}, \mathbf{b}, \mathbf{c}\) form a complete right-handed basis. These restrictions impose no loss of generality, since it is possible to rotate/invert any set of 3 crystal basis vectors so that they conform to the restrictions.

For example, assume that the 3 vectors \(\mathbf{A}, \mathbf{B}, \mathbf{C}\) are the edge vectors of a general parallelepiped, where there is no restriction on \(\mathbf{A}, \mathbf{B}, \mathbf{C}\) other than they form a complete right-handed basis i.e. \(\mathbf{A} \times \mathbf{B} \times \mathbf{C} > 0\). The equivalent LAMMPS \(\mathbf{a}, \mathbf{b}, \mathbf{c}\) are a linear rotation of \(\mathbf{A}, \mathbf{B}, \mathbf{C}\) and can be computed as follows:
\[
\begin{pmatrix}
a & b & c \\
\end{pmatrix} = \begin{pmatrix}
a_x & b_x & c_x \\
0 & b_y & c_y \\
0 & 0 & c_z \\
\end{pmatrix}
\]

\[
a_x = A
\]

\[
b_x = B \cdot \hat{A} = B \cos \gamma
\]

\[
b_y = |\hat{A} \times B| = B \sin \gamma = \sqrt{B^2 - b_x^2}
\]

\[
c_x = C \cdot \hat{A} = C \cos \beta
\]

\[
c_y = C \cdot (A \times B) \times \hat{A} = \frac{B \cdot C - b_x c_x}{b_y}
\]

\[
c_z = |C \cdot (A \times B)| = \sqrt{C^2 - c_x^2 - c_y^2}
\]

where \( A = |A| \) indicates the scalar length of \( A \). The ^ hat symbol indicates the corresponding unit vector. \( \beta \) and \( \gamma \) are angles between the vectors described below. Note that by construction, \( a, b, \) and \( c \) have strictly positive x, y, and z components, respectively. If it should happen that \( A, B, \) and \( C \) form a left-handed basis, then the above equations are not valid for \( c \). In this case, it is necessary to first apply an inversion. This can be achieved by interchanging two basis vectors or by changing the sign of one of them.

For consistency, the same rotation/inversion applied to the basis vectors must also be applied to atom positions, velocities, and any other vector quantities. This can be conveniently achieved by first converting to fractional coordinates in the old basis and then converting to distance coordinates in the new basis. The transformation is given by the following equation:

\[
x = (a \ b \ c) \cdot \frac{1}{V} \begin{pmatrix} B \times C \\ C \times A \\ A \times B \end{pmatrix} \cdot X
\]

where \( V \) is the volume of the box, \( X \) is the original vector quantity and \( x \) is the vector in the LAMMPS basis.

There is no requirement that a triclinic box be periodic in any dimension, though it typically should be in at least the 2nd dimension of the tilt (y in xy) if you want to enforce a shift in periodic boundary conditions across that
boundary. Some commands that work with triclinic boxes, e.g. the fix deform and fix npt commands, require periodicity or non-shrink-wrap boundary conditions in specific dimensions. See the command doc pages for details.

The 9 parameters (xlo,xhi,ylo,yhi,zlo,zhi,xy,xz,yz) are defined at the time the simulation box is created. This happens in one of 3 ways. If the create_box command is used with a region of style prism, then a triclinic box is setup. See the region command for details. If the read_data command is used to define the simulation box, and the header of the data file contains a line with the "xy xz yz" keyword, then a triclinic box is setup. See the read_data command for details. Finally, if the read_restart command reads a restart file which was written from a simulation using a triclinic box, then a triclinic box will be setup for the restarted simulation.

Note that you can define a triclinic box with all 3 tilt factors = 0.0, so that it is initially orthogonal. This is necessary if the box will become non-orthogonal, e.g. due to the fix npt or fix deform commands. Alternatively, you can use the change_box command to convert a simulation box from orthogonal to triclinic and vice versa.

As with orthogonal boxes, LAMMPS defines triclinic box size parameters lx,ly,lz where lx = xhi-xlo, and similarly in the y and z dimensions. The 9 parameters, as well as lx,ly,lz, can be output via the thermo_style custom command.

To avoid extremely tilted boxes (which would be computationally inefficient), LAMMPS normally requires that no tilt factor can skew the box more than half the distance of the parallel box length, which is the 1st dimension in the tilt factor (x for xz). This is required both when the simulation box is created, e.g. via the create_box or read_data commands, as well as when the box shape changes dynamically during a simulation, e.g. via the fix deform or fix npt commands.

For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are geometrically all equivalent. If the box tilt exceeds this limit during a dynamics run (e.g. via the fix deform command), then the box is "flipped" to an equivalent shape with a tilt factor within the bounds, so the run can continue. See the fix deform doc page for further details.

One exception to this rule is if the 1st dimension in the tilt factor (x for xy) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient, due to the highly skewed simulation box.

The limitation on not creating a simulation box with a tilt factor skewing the box more than half the distance of the parallel box length can be overridden via the box command. Setting the tilt keyword to large allows any tilt factors to be specified.

Box flips that may occur using the fix deform or fix npt commands can be turned off using the flip no option with either of the commands.

Note that if a simulation box has a large tilt factor, LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

Triclinic crystal structures are often defined using three lattice constants a, b, and c, and three angles alpha, beta and gamma. Note that in this nomenclature, the a, b, and c lattice constants are the scalar lengths of the edge vectors a, b, and c defined above. The relationship between these 6 quantities (a,b,c,alpha,beta,gamma) and the LAMMPS box sizes (lx,ly,lz) = (xhi-xlo,yhi-ylo,zhi-zlo) and tilt factors (xy,xz,yz) is as follows:
\[ a = lx \]
\[ b^2 = ly^2 + xy^2 \]
\[ c^2 = l z^2 + xz^2 + yz^2 \]
\[ \cos \alpha = \frac{xy \cdot xz + ly \cdot yz}{b \cdot c} \]
\[ \cos \beta = \frac{xz}{c} \]
\[ \cos \gamma = \frac{xy}{b} \]

The inverse relationship can be written as follows:

\[ lx = a \]
\[ xy = b \cos \gamma \]
\[ xz = c \cos \beta \]
\[ ly^2 = b^2 - xy^2 \]
\[ yz = \frac{b \cdot c \cos \alpha - xy \cdot xz}{ly} \]
\[ l z^2 = c^2 - xz^2 - yz^2 \]

The values of \(a, b, c, \alpha, \beta, \) and \(\gamma\) can be printed out or accessed by computes using the thermo_style custom keywords cella, cellb, ccell, cellalpha, cellbeta, cellgamma, respectively.

As discussed on the dump command doc page, when the BOX BOUNDS for a snapshot is written to a dump file for a triclinic box, an orthogonal bounding box which encloses the triclinic simulation box is output, along with the 3 tilt factors (\(xy, xz, yz\)) of the triclinic box, formatted as follows:

\[ \text{ITEM: BOX BOUNDS xy xz yz} \]
\[ xlo \_bound \ xhi \_bound \ xy \]
\[ ylo \_bound \ yhi \_bound \ xz \]
\[ zlo \_bound \ zhi \_bound \ yz \]

This bounding box is convenient for many visualization programs and is calculated from the 9 triclinic box parameters (\(xlo, xhi, ylo, yhi, zlo, zhi, xy, xz, yz\)) as follows:

\[ xlo \_bound = xlo + \text{MIN}(0.0, xy, xz, xy+xz) \]
\[ xhi \_bound = xhi + \text{MAX}(0.0, xy, xz, xy+xz) \]
\[ ylo \_bound = ylo + \text{MIN}(0.0, yz) \]
These formulas can be inverted if you need to convert the bounding box back into the triclinic box parameters, e.g. $x_{lo} = x_{lo\_bound} - \min(0.0, xy, xz, xy+xz)$.

One use of triclinic simulation boxes is to model solid-state crystals with triclinic symmetry. The `lattice` command can be used with non-orthogonal basis vectors to define a lattice that will tile a triclinic simulation box via the `create_atoms` command.

A second use is to run Parinello-Rahman dynamics via the `fix npt` command, which will adjust the $xy$, $xz$, $yz$ tilt factors to compensate for off-diagonal components of the pressure tensor. The analog for an energy minimization is the `fix box/relax` command.

A third use is to shear a bulk solid to study the response of the material. The `fix deform` command can be used for this purpose. It allows dynamic control of the $xy$, $xz$, $yz$ tilt factors as a simulation runs. This is discussed in the next section on non-equilibrium MD (NEMD) simulations.

### 6.13 NEMD simulations

Non-equilibrium molecular dynamics or NEMD simulations are typically used to measure a fluid's rheological properties such as viscosity. In LAMMPS, such simulations can be performed by first setting up a non-orthogonal simulation box (see the preceding Howto section).

A shear strain can be applied to the simulation box at a desired strain rate by using the `fix deform` command. The `fix nvt/sllod` command can be used to thermostat the sheared fluid and integrate the SLLOD equations of motion for the system. Fix nvt/sllod uses `compute temp/deform` to compute a thermal temperature by subtracting out the streaming velocity of the shearing atoms. The velocity profile or other properties of the fluid can be monitored via the `fix ave/spatial` command.

As discussed in the previous section on non-orthogonal simulation boxes, the amount of tilt or skew that can be applied is limited by LAMMPS for computational efficiency to be $1/2$ of the parallel box length. However, `fix deform` can continuously strain a box by an arbitrary amount. As discussed in the `fix deform` command, when the tilt value reaches a limit, the box is flipped to the opposite limit which is an equivalent tiling of periodic space. The strain rate can then continue to change as before. In a long NEMD simulation these box re-shaping events may occur many times.

In a NEMD simulation, the "remap" option of `fix deform` should be set to "remap v", since that is what `fix nvt/sllod` assumes to generate a velocity profile consistent with the applied shear strain rate.

An alternative method for calculating viscosities is provided via the `fix viscosity` command.

### 6.14 Extended spherical and aspherical particles

Typical MD models treat atoms or particles as point masses. Sometimes, however, it is desirable to have a model with finite-size particles such as spheres or aspherical ellipsoids. The difference is that such particles have a moment of inertia, rotational energy, and angular momentum. Rotation is induced by torque from interactions with other particles.
LAMMPS has several options for running simulations with these kinds of particles. The following aspects are discussed in turn:

- atom styles
- pair potentials
- time integration
- computes, thermodynamics, and dump output
- rigid bodies composed of extended particles

Atom styles

There are 2 atom styles that allow for definition of finite-size particles: sphere and ellipsoid. The peri atom style also treats particles as having a volume, but that is internal to the pair_style peri potentials. The dipole atom style is most often used in conjunction with finite-size particles.

The sphere style defines particles that are spheroids and each particle can have a unique diameter and mass (or density). These particles store an angular velocity (omega) and can be acted upon by torque. The "set" command can be used to modify the diameter and mass of individual particles, after they are created.

The ellipsoid style defines particles that are ellipsoids and thus can be aspherical. Each particle has a shape, specified by 3 diameters, and mass (or density). These particles store an angular momentum and their orientation (quaternion), and can be acted upon by torque. They do not store an angular velocity (omega), which can be in a different direction than angular momentum, rather they compute it as needed. The "set" command can be used to modify the diameter, orientation, and mass of individual particles, after they are created. It also has a brief explanation of what quaternions are.

The dipole style does not define extended particles, but is often used in conjunction with spherical particles, via a command like

atom_style hybrid sphere dipole

This is because when dipoles interact with each other, they induce torques, and a particle must be extended (i.e. have a moment of inertia) in order to respond and rotate. See the atom_style dipole command for details. The "set" command can be used to modify the orientation and length of the dipole moment of individual particles, after they are created.

Note that if one of these atom styles is used (or multiple styles via the atom_style hybrid command), not all particles in the system are required to be finite-size or aspherical. For example, if the 3 shape parameters are set to the same value, the particle will be a sphere rather than an ellipsoid. If the 3 shape parameters are all set to 0.0 or if the diameter is set to 0.0, it will be a point particle. If the length of the dipole moment is set to zero, the particle will not have a point dipole associated with it. The pair styles used to compute pairwise interactions will typically compute the correct interaction in these simplified (cheaper) cases. Pair_style hybrid can be used to insure the correct interactions are computed for the appropriate style of interactions. Likewise, using groups to partition particles (ellipsoids versus spheres versus point particles) will allow you to use the appropriate time integrators and temperature computations for each class of particles. See the doc pages for various commands for details.

Also note that for 2d simulations, finite-size spheres and ellipsoids are still treated as 3d particles, rather than as circular disks or ellipses. This means they have the same moment of inertia for a 3d extended object. When their temperature is cocomputed, the correct degrees of freedom are used for rotation in a 2d versus 3d system.
**Pair potentials**

When a system with extended particles is defined, the particles will only rotate and experience torque if the force field computes such interactions. These are the various pair styles that generate torque:

- `pair_style gran/history`
- `pair_style gran/hertzian`
- `pair_style gran/no_history`
- `pair_style dipole/cut`
- `pair_style gayberne`
- `pair_style resquared`
- `pair_style lubricate`

The granular pair styles are used with spherical particles. The dipole pair style is used with atom_style dipole, which could be applied to spherical or ellipsoidal particles. The GayBerne and REsquared potentials require ellipsoidal particles, though they will also work if the 3 shape parameters are the same (a sphere). The lubrication potential works with spherical particles.

**Time integration**

There are 3 fixes that perform time integration on extended spherical particles, meaning the integrators update the rotational orientation and angular velocity or angular momentum of the particles:

- `fix nve/sphere`
- `fix nvt/sphere`
- `fix npt/sphere`

Likewise, there are 3 fixes that perform time integration on ellipsoids as extended aspherical particles:

- `fix nve/asphere`
- `fix nvt/asphere`
- `fix npt/asphere`

The advantage of these fixes is that those which thermostat the particles include the rotational degrees of freedom in the temperature calculation and thermostating. Other thermostats can be used with fix nve/sphere or fix nve/asphere, such as fix langevin or fix temp/berendsen, but those thermostats only operate on the translational kinetic energy of the extended particles.

Note that for mixtures of point and extended particles, you should only use these integration fixes on groups which contain extended particles.

**Computes, thermodynamics, and dump output**

There are 4 computes that calculate the temperature or rotational energy of extended spherical or aspherical particles (ellipsoids):

- `compute temp/sphere`
- `compute temp/asphere`
- `compute erotate/sphere`
- `compute erotate/asphere`

These include rotational degrees of freedom in their computation. If you wish the thermodynamic output of temperature or pressure to use one of these computes (e.g. for a system entirely composed of extended particles),
then the compute can be defined and the `thermo_modify` command used. Note that by default thermodynamic quantities will be calculated with a temperature that only includes translational degrees of freedom. See the `thermo_style` command for details.

The `dump custom` command can output various attributes of extended particles, including the dipole moment (mu), the angular velocity (omega), the angular momentum (angmom), the quaternion (quat), and the torque (tq) on the particle.

**Rigid bodies composed of extended particles**

The `fix rigid` command treats a collection of particles as a rigid body, computes its inertia tensor, sums the total force and torque on the rigid body each timestep due to forces on its constituent particles, and integrates the motion of the rigid body.

If any of the constituent particles of a rigid body are extended particles (spheres or ellipsoids), then their contribution to the inertia tensor of the body is different than if they were point particles. This means the rotational dynamics of the rigid body will be different. Thus a model of a dimer is different if the dimer consists of two point masses versus two extended spheroids, even if the two particles have the same mass. Extended particles that experience torque due to their interaction with other particles will also impart that torque to a rigid body they are part of.

See the "fix rigid" command for example of complex rigid-body models it is possible to define in LAMMPS.

Note that the `fix shake` command can also be used to treat 2, 3, or 4 particles as a rigid body, but it always assumes the particles are point masses.

### 6.15 Output from LAMMPS (thermo, dumps, computes, fixes, variables)

There are four basic kinds of LAMMPS output:

- **Thermodynamic output**, which is a list of quantities printed every few timesteps to the screen and logfile.
- **Dump files**, which contain snapshots of atoms and various per-atom values and are written at a specified frequency.
- Certain fixes can output user-specified quantities to files: `fix ave/time` for time averaging, `fix ave/spatial` for spatial averaging, and `fix print` for single-line output of variables. Fix print can also output to the screen.
- **Restart files**.

A simulation prints one set of thermodynamic output and (optionally) restart files. It can generate any number of dump files and fix output files, depending on what `dump` and `fix` commands you specify.

As discussed below, LAMMPS gives you a variety of ways to determine what quantities are computed and printed when the thermodynamics, dump, or fix commands listed above perform output. Throughout this discussion, note that users can also add their own computes and fixes to LAMMPS which can then generate values that can then be output with these commands.

The following sub-sections discuss different LAMMPS command related to output and the kind of data they operate on and produce:

- **Global/per-atom/local data**
- **Scalar/vector/array data**
• Thermodynamic output
• Dump file output
• Fixes that write output files
• Computes that process output quantities
• Fixes that process output quantities
• Computes that generate values to output
• Fixes that generate values to output
• Variables that generate values to output
• Summary table of output options and data flow between commands

Global/per-atom/local data

Various output-related commands work with three different styles of data: global, per-atom, or local. A global datum is one or more system-wide values, e.g. the temperature of the system. A per-atom datum is one or more values per atom, e.g. the kinetic energy of each atom. Local datums are calculated by each processor based on the atoms it owns, but there may be zero or more per atom, e.g. a list of bond distances.

Scalar/vector/array data

Global, per-atom, and local datums can each come in three kinds: a single scalar value, a vector of values, or a 2d array of values. The doc page for a "compute" or "fix" or "variable" that generates data will specify both the style and kind of data it produces, e.g. a per-atom vector.

When a quantity is accessed, as in many of the output commands discussed below, it can be referenced via the following bracket notation, where ID in this case is the ID of a compute. The leading "c_" would be replaced by "f_" for a fix, or "v_" for a variable:

<table>
<thead>
<tr>
<th>Notation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>c_ID</td>
<td>entire scalar, vector, or array</td>
</tr>
<tr>
<td>c_ID[I]</td>
<td>one element of vector, one column of array</td>
</tr>
<tr>
<td>c_ID[I][J]</td>
<td>one element of array</td>
</tr>
</tbody>
</table>

In other words, using one bracket reduces the dimension of the data once (vector -> scalar, array -> vector). Using two brackets reduces the dimension twice (array -> scalar). Thus a command that uses scalar values as input can typically also process elements of a vector or array.

Thermodynamic output

The frequency and format of thermodynamic output is set by the thermo, thermo_style, and thermo_modify commands. The thermo_style command also specifies what values are calculated and written out. Pre-defined keywords can be specified (e.g. press, etotal, etc). Three additional kinds of keywords can also be specified (c_ID, f_ID, v_name), where a compute or fix or variable provides the value to be output. In each case, the compute, fix, or variable must generate global values for input to the thermo_style custom command.

Dump file output

Dump file output is specified by the dump and dump_modify commands. There are several pre-defined formats (dump atom, dump xtc, etc).

There is also a dump custom format where the user specifies what values are output with each atom. Pre-defined atom attributes can be specified (id, x, fx, etc). Three additional kinds of keywords can also be specified (c_ID, f_ID, v_name), where a compute or fix or variable provides the values to be output. In each case, the compute, fix, or variable must generate per-atom values for input to the dump custom command.
There is also a dump local format where the user specifies what local values to output. A pre-defined index keyword can be specified to enumerate the local values. Two additional kinds of keywords can also be specified (c_ID, f_ID), where a compute or fix or variable provides the values to be output. In each case, the compute or fix must generate local values for input to the dump local command.

**Fixes that write output files**

Several fixes take various quantities as input and can write output files: fix ave/time, fix ave/spatial, fix ave/histo, fix ave/correlate, and fix print.

The fix ave/time command enables direct output to a file and/or time-averaging of global scalars or vectors. The user specifies one or more quantities as input. These can be global compute values, global fix values, or variables of any style except the atom style which produces per-atom values. Since a variable can refer to keywords used by the thermo_style custom command (like temp or press) and individual per-atom values, a wide variety of quantities can be time averaged and/or output in this way. If the inputs are one or more scalar values, then the fix generates a global scalar or vector of output. If the inputs are one or more vector values, then the fix generates a global vector or array of output. The time-averaged output of this fix can also be used as input to other output commands.

The fix ave/spatial command enables direct output to a file of spatial-averaged per-atom quantities like those output in dump files, within 1d layers of the simulation box. The per-atom quantities can be atom density (mass or number) or atom attributes such as position, velocity, force. They can also be per-atom quantities calculated by a compute, by a fix, or by an atom-style variable. The spatial-averaged output of this fix can also be used as input to other output commands.

The fix ave/histo command enables direct output to a file of histogrammed quantities, which can be global or per-atom or local quantities. The histogram output of this fix can also be used as input to other output commands.

The fix ave/correlate command enables direct output to a file of time-correlated quantities, which can be global scalars. The correlation matrix output of this fix can also be used as input to other output commands.

The fix print command can generate a line of output written to the screen and log file or to a separate file, periodically during a running simulation. The line can contain one or more variable values for any style variable except the atom style. As explained above, variables themselves can contain references to global values generated by thermodynamic keywords, computes, fixes, or other variables, or to per-atom values for a specific atom. Thus the fix print command is a means to output a wide variety of quantities separate from normal thermodynamic or dump file output.

**Computes that process output quantities**

The compute reduce and compute reduce/region commands take one or more per-atom or local vector quantities as inputs and "reduce" them (sum, min, max, ave) to scalar quantities. These are produced as output values which can be used as input to other output commands.

The compute slice command takes one or more global vector or array quantities as inputs and extracts a subset of their values to create a new vector or array. These are produced as output values which can be used as input to other output commands.

The compute property/atom command takes a list of one or more pre-defined atom attributes (id, x, fx, etc) and stores the values in a per-atom vector or array. These are produced as output values which can be used as input to other output commands. The list of atom attributes is the same as for the dump custom command.
The compute property/local command takes a list of one or more pre-defined local attributes (bond info, angle info, etc) and stores the values in a local vector or array. These are produced as output values which can be used as input to other output commands.

The compute atom/molecule command takes a list of one or more per-atom quantities (from a compute, fix, per-atom variable) and sums the quantities on a per-molecule basis. It produces a global vector or array as output values which can be used as input to other output commands.

Fixes that process output quantities

The fix ave/atom command performs time-averaging of per-atom vectors. The per-atom quantities can be atom attributes such as position, velocity, force. They can also be per-atom quantities calculated by a compute, by a fix, or by an atom-style variable. The time-averaged per-atom output of this fix can be used as input to other output commands.

The fix store/state command can archive one or more per-atom attributes at a particular time, so that the old values can be used in a future calculation or output. The list of atom attributes is the same as for the dump custom command, including per-atom quantities calculated by a compute, by a fix, or by an atom-style variable. The output of this fix can be used as input to other output commands.

Computes that generate values to output

Every compute in LAMMPS produces either global or per-atom or local values. The values can be scalars or vectors or arrays of data. These values can be output using the other commands described in this section. The doc page for each compute command describes what it produces. Computes that produce per-atom or local values have the word "atom" or "local" in their style name. Computes without the word "atom" or "local" produce global values.

Fixes that generate values to output

Some fixes in LAMMPS produces either global or per-atom or local values which can be accessed by other commands. The values can be scalars or vectors or arrays of data. These values can be output using the other commands described in this section. The doc page for each fix command tells whether it produces any output quantities and describes them.

Variables that generate values to output

Every variables defined in an input script generates either a global scalar value or a per-atom vector (only atom-style variables) when it is accessed. The formulas used to define equal- and atom-style variables can contain references to the thermodynamic keywords and to global and per-atom data generated by computes, fixes, and other variables. The values generated by variables can be output using the other commands described in this section.

Summary table of output options and data flow between commands

This table summarizes the various commands that can be used for generating output from LAMMPS. Each command produces output data of some kind and/or writes data to a file. Most of the commands can take data from other commands as input. Thus you can link many of these commands together in pipeline form, where data produced by one command is used as input to another command and eventually written to the screen or to a file. Note that to hook two commands together the output and input data types must match, e.g. global/per-atom/local data and scalar/vector/array data.
Also note that, as described above, when a command takes a scalar as input, that could be an element of a vector or array. Likewise a vector input could be a column of an array.

<table>
<thead>
<tr>
<th>Command</th>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>thermo_style custom</td>
<td>global scalars</td>
<td>screen, log file</td>
</tr>
<tr>
<td>dump custom</td>
<td>per-atom vectors</td>
<td>dump file</td>
</tr>
<tr>
<td>dump local</td>
<td>local vectors</td>
<td>dump file</td>
</tr>
<tr>
<td>fix print</td>
<td>global scalar from variable</td>
<td>screen, file</td>
</tr>
<tr>
<td>print</td>
<td>global scalar from variable</td>
<td>screen</td>
</tr>
<tr>
<td>computes</td>
<td>N/A</td>
<td>global/per-atom/local scalar/vector/array</td>
</tr>
<tr>
<td>fixes</td>
<td>N/A</td>
<td>global/per-atom/local scalar/vector/array</td>
</tr>
<tr>
<td>variables</td>
<td>global scalars, per-atom vectors</td>
<td>global scalar, per-atom vector</td>
</tr>
<tr>
<td>compute reduce</td>
<td>per-atom/local vectors</td>
<td>global scalar/vector</td>
</tr>
<tr>
<td>compute slice</td>
<td>global vectors/arrays</td>
<td>global vector/array</td>
</tr>
<tr>
<td>compute property/atom</td>
<td>per-atom vectors</td>
<td>per-atom vector/array</td>
</tr>
<tr>
<td>compute property/local</td>
<td>local vectors</td>
<td>local vector/array</td>
</tr>
<tr>
<td>compute atom/molecule</td>
<td>per-atom vectors</td>
<td>global vector/array</td>
</tr>
<tr>
<td>fix ave/atom</td>
<td>per-atom vectors</td>
<td>per-atom vector/array</td>
</tr>
<tr>
<td>fix ave/time</td>
<td>global scalars/vecors</td>
<td>global scalar/vector/array, file</td>
</tr>
<tr>
<td>fix ave/spatial</td>
<td>per-atom vectors</td>
<td>global array, file</td>
</tr>
<tr>
<td>fix ave/histo</td>
<td>global/per-atom/local scalars and vectors</td>
<td>global array, file</td>
</tr>
<tr>
<td>fix ave/correlate</td>
<td>global scalars</td>
<td>global array, file</td>
</tr>
<tr>
<td>fix store/state</td>
<td>per-atom vectors</td>
<td>per-atom vector/array</td>
</tr>
</tbody>
</table>

6.16 Thermostatting, barostatting, and computing temperature

Thermostatting means controlling the temperature of particles in an MD simulation. Barostatting means controlling the pressure. Since the pressure includes a kinetic component due to particle velocities, both these operations require calculation of the temperature. Typically a target temperature (T) and/or pressure (P) is specified by the user, and the thermostat or barostat attempts to equilibrate the system to the requested T and/or P.

Temperature is computed as kinetic energy divided by some number of degrees of freedom (and the Boltzmann constant). Since kinetic energy is a function of particle velocity, there is often a need to distinguish between a particle's advection velocity (due to some aggregate motion of particles) and its thermal velocity. The sum of the two is the particle's total velocity, but the latter is often what is wanted to compute a temperature.

LAMMPS has several options for computing temperatures, any of which can be used in thermostatting and barostatting. These compute commands calculate temperature, and the compute pressure command calculates pressure.

- compute temp
- compute temp/sphere
- compute temp/asphere
- compute temp/com
- compute temp/deform
- compute temp/partial
- compute temp/profile
• compute temp/ramp
• compute temp/region

All but the first 3 calculate velocity biases (i.e. advection velocities) that are removed when computing the thermal temperature. Compute temp/sphere and compute temp/asphere compute kinetic energy for extended particles that includes rotational degrees of freedom. They both allow, as an extra argument, which is another temperature compute that subtracts a velocity bias. This allows the translational velocity of extended spherical or aspherical particles to be adjusted in prescribed ways.

Thermostatting in LAMMPS is performed by fixes, or in one case by a pair style. Four thermostatting fixes are currently available: Nose-Hoover (nvt), Berendsen, Langevin, and direct rescaling (temp/rescale). Dissipative particle dynamics (DPD) thermostatting can be invoked via the dpd/tstat pair style:

• fix nvt
• fix nvt/sphere
• fix nvt/asphere
• fix nvt/sllod
• fix temp/berendsen
• fix langevin
• fix temp/rescale
• pair_style dpd/tstat

Fix nvt only thermostats the translational velocity of particles. Fix nvt/sllod also does this, except that it subtracts out a velocity bias due to a deforming box and integrates the SLLOD equations of motion. See the NEMD simulations section of this page for further details. Fix nvt/sphere and fix nvt/asphere thermostat not only translation velocities but also rotational velocities for spherical and aspherical particles.

DPD thermostatting alters pairwise interactions in a manner analogous to the per-particle thermostatting of fix langevin.

Any of the thermostatting fixes can use temperature computes that remove bias for two purposes: (a) computing the current temperature to compare to the requested target temperature, and (b) adjusting only the thermal temperature component of the particle's velocities. See the doc pages for the individual fixes and for the fix_modify command for instructions on how to assign a temperature compute to a thermostatting fix. For example, you can apply a thermostat to only the x and z components of velocity by using it in conjunction with compute temp/partial.

IMPORTANT NOTE: Only the nvt fixes perform time integration, meaning they update the velocities and positions of particles due to forces and velocities respectively. The other thermostat fixes only adjust velocities; they do NOT perform time integration updates. Thus they should be used in conjunction with a constant NVE integration fix such as these:

• fix nve
• fix nve/sphere
• fix nve/asphere

Barostatting in LAMMPS is also performed by fixes. Two barostatting methods are currently available: Nose-Hoover (npt and nph) and Berendsen:

• fix npt
• fix npt/sphere
• fix npt/asphere
The `fix npt` commands include a Nose-Hoover thermostat and barostat. *Fix nph* is just a Nose/Hoover barostat; it does no thermostatting. Both `fix nph` and `fix press/berendsen` can be used in conjunction with any of the thermostating fixes.

As with the thermostats, `fix npt` and `fix nph` only use translational motion of the particles in computing T and P and performing thermo/barostatting. *Fix npt/sphere* and *fix npt/asphere* thermo/barostat using not only translation velocities but also rotational velocities for spherical and aspherical particles.

All of the barostatting fixes use the `compute pressure` compute to calculate a current pressure. By default, this compute is created with a simple `compute temp` (see the last argument of the `compute pressure` command), which is used to calculated the kinetic componenet of the pressure. The barostatting fixes can also use temperature computes that remove bias for the purpose of computing the kinetic componenet which contributes to the current pressure. See the doc pages for the individual fixes and for the `fix_modify` command for instructions on how to assign a temperature or pressure compute to a barostatting fix.

**IMPORTANT NOTE:** As with the thermostats, the Nose/Hoover methods (*fix npt* and *fix nph*) perform time integration. *Fix press/berendsen* does NOT, so it should be used with one of the constant NVE fixes or with one of the NVT fixes.

Finally, thermodynamic output, which can be setup via the `thermo_style` command, often includes temperature and pressure values. As explained on the doc page for the `thermo_style` command, the default T and P are setup by the thermo command itself. They are NOT the ones associated with any thermostatting or barostatting fix you have defined or with any compute that calculates a temperature or pressure. Thus if you want to view these values of T and P, you need to specify them explicitly via a `thermo_style custom` command. Or you can use the `thermo_modify` command to re-define what temperature or pressure compute is used for default thermodynamic output.

### 6.17 Walls

Walls in an MD simulation are typically used to bound particle motion, i.e. to serve as a boundary condition.

Walls in LAMMPS can be of rough (made of particles) or idealized surfaces. Ideal walls can be smooth, generating forces only in the normal direction, or frictional, generating forces also in the tangential direction.

Rough walls, built of particles, can be created in various ways. The particles themselves can be generated like any other particle, via the `lattice` and `create_atoms` commands, or read in via the `read_data` command.

Their motion can be constrained by many different commands, so that they do not move at all, move together as a group at constant velocity or in response to a net force acting on them, move in a prescribed fashion (e.g. rotate around a point), etc. Note that if a time integration fix like `fix nve` or `fix nvt` is not used with the group that contains wall particles, their positions and velocities will not be updated.

- `fix aveforce` - set force on particles to average value, so they move together
- `fix setforce` - set force on particles to a value, e.g. 0.0
- `fix freeze` - freeze particles for use as granular walls
- `fix nve/noforce` - advect particles by their velocity, but without force
- `fix move` - prescribe motion of particles by a linear velocity, oscillation, rotation, variable
The **fix move** command offers the most generality, since the motion of individual particles can be specified with **variable** formula which depends on time and/or the particle position.

For rough walls, it may be useful to turn off pairwise interactions between wall particles via the **neigh_modify exclude** command.

Rough walls can also be created by specifying frozen particles that do not move and do not interact with mobile particles, and then tethering other particles to the fixed particles, via a **bond**. The bonded particles do interact with other mobile particles.

Idealized walls can be specified via several fix commands. **Fix wall/gran** creates frictional walls for use with granular particles; all the other commands create smooth walls.

- **fix wall/reflect** - reflective flat walls
- **fix wall/lj93** - flat walls, with Lennard-Jones 9/3 potential
- **fix wall/lj126** - flat walls, with Lennard-Jones 12/6 potential
- **fix wall/collloid** - flat walls, with pair_style colloid potential
- **fix wall/harmonic** - flat walls, with repulsive harmonic spring potential
- **fix wall/region** - use region surface as wall
- **fix wall/gran** - flat or curved walls with pair_style granular potential

The **lj93, lj126, colloid, and harmonic** styles all allow the flat walls to move with a constant velocity, or oscillate in time. The **fix wall/region** command offers the most generality, since the region surface is treated as a wall, and the geometry of the region can be a simple primitive volume (e.g. a sphere, or cube, or plane), or a complex volume made from the union and intersection of primitive volumes. **Regions** can also specify a volume "interior" or "exterior" to the specified primitive shape or union or intersection. **Regions** can also be "dynamic" meaning they move with constant velocity, oscillate, or rotate.

The only frictional idealized walls currently in LAMMPS are flat or curved surfaces specified by the **fix wall/gran** command. At some point we plan to allow region surfaces to be used as frictional walls, as well as triangulated surfaces.

### 6.18 Elastic constants

Elastic constants characterize the stiffness of a material. The formal definition is provided by the linear relation that holds between the stress and strain tensors in the limit of infinitesimal deformation. In tensor notation, this is expressed as \( s_{ij} = C_{ijkl} \times e_{kl} \), where the repeated indices imply summation. \( s_{ij} \) are the elements of the symmetric stress tensor. \( e_{kl} \) are the elements of the symmetric strain tensor. \( C_{ijkl} \) are the elements of the fourth rank tensor of elastic constants. In three dimensions, this tensor has \( 3^4 = 81 \) elements. Using Voigt notation, the tensor can be written as a 6x6 matrix, where \( C_{ij} \) is now the derivative of \( s_i \) w.r.t. \( e_j \). Because \( s_i \) is itself a derivative w.r.t. \( e_i \), it follows that \( C_{ij} \) is also symmetric, with at most \( 7 \times 6/2 = 21 \) distinct elements.

At zero temperature, it is easy to estimate these derivatives by deforming the simulation box in one of the six directions using the **change_box** command and measuring the change in the stress tensor. A general-purpose script that does this is given in the examples/elastic directory described in this section.

Calculating elastic constants at finite temperature is more challenging, because it is necessary to run a simulation that performs time averages of differential properties. One way to do this is to measure the change in average stress tensor in an NVT simulations when the cell volume undergoes a finite deformation. In order to balance the systematic and statistical errors in this method, the magnitude of the deformation must be chosen judiciously, and care must be taken to fully equilibrate the deformed cell before sampling the stress tensor. Another approach is to
sample the triclinic cell fluctuations that occur in an NPT simulation. This method can also be slow to converge and requires careful post-processing (Shinoda)

### 6.19 Library interface to LAMMPS

As described in Section start 4, LAMMPS can be built as a library, so that it can be called by another code, used in a coupled manner with other codes, or driven through a Python interface.

All of these methodologies use a C-style interface to LAMMPS that is provided in the files src/library.cpp and src/library.h. The functions therein have a C-style argument list, but contain C++ code you could write yourself in a C++ application that was invoking LAMMPS directly. The C++ code in the functions illustrates how to invoke internal LAMMPS operations. Note that LAMMPS classes are defined within a LAMMPS namespace (LAMMPS_NS) if you use them from another C++ application.

Library.cpp contains these 4 functions:

```cpp
void lammps_open(int, char **, MPI_Comm, void **);
void lammps_close(void *);
void lammps_file(void *, char *);
char *lammps_command(void *, char *);
```

The `lammps_open()` function is used to initialize LAMMPS, passing in a list of strings as if they were command-line arguments when LAMMPS is run in stand-alone mode from the command line, and a MPI communicator for LAMMPS to run under. It returns a ptr to the LAMMPS object that is created, and which is used in subsequent library calls. The `lammps_open()` function can be called multiple times, to create multiple instances of LAMMPS.

LAMMPS will run on the set of processors in the communicator. This means the calling code can run LAMMPS on all or a subset of processors. For example, a wrapper script might decide to alternate between LAMMPS and another code, allowing them both to run on all the processors. Or it might allocate half the processors to LAMMPS and half to the other code and run both codes simultaneously before syncing them up periodically. Or it might instantiate multiple instances of LAMMPS to perform different calculations.

The `lammps_close()` function is used to shut down an instance of LAMMPS and free all its memory.

The `lammps_file()` and `lammps_command()` functions are used to pass a file or string to LAMMPS as if it were an input script or single command in an input script. Thus the calling code can read or generate a series of LAMMPS commands one at a time and pass it thru the library interface to setup a problem and then run it, interleaving the `lammps_command()` calls with other calls to extract information from LAMMPS, perform its own operations, or call another code's library.

Other useful functions are also included in library.cpp. For example:

```cpp
void *lammps_extract_global(void *, char *)
void *lammps_extract_atom(void *, char *)
void *lammps_extract_compute(void *, char *, int, int)
void *lammps_extract_fix(void *, char *, int, int, int, int)
void *lammps_extract_variable(void *, char *, char *)
int lammps_get_natoms(void *)
void lammps_get_coords(void *, double *)
void lammps_put_coords(void *, double *)
```

These can extract various global or per-atom quantities from LAMMPS as well as values calculated by a
compute, fix, or variable. The "get" and "put" operations can retrieve and reset atom coordinates. See the library.cpp file and its associated header file library.h for details.

The key idea of the library interface is that you can write any functions you wish to define how your code talks to LAMMPS and add them to src/library.cpp and src/library.h, as well as to the Python interface. The routines you add can access or change any LAMMPS data you wish. The examples/COUPLE and python directories have example C++ and C and Python codes which show how a driver code can link to LAMMPS as a library, run LAMMPS on a subset of processors, grab data from LAMMPS, change it, and put it back into LAMMPS.

6.20 Calculating thermal conductivity

The thermal conductivity kappa of a material can be measured in at least 3 ways using various options in LAMMPS. (See this section of the manual for an analogous discussion for viscosity). The thermal conductivity tensor kappa is a measure of the propensity of a material to transmit heat energy in a diffusive manner as given by Fourier's law

\[ J = -\kappa \text{grad}(T) \]

where J is the heat flux in units of energy per area per time and grad(T) is the spatial gradient of temperature. The thermal conductivity thus has units of energy per distance per time per degree K and is often approximated as an isotropic quantity, i.e. as a scalar.

The first method is to setup two thermostatted regions at opposite ends of a simulation box, or one in the middle and one at the end of a periodic box. By holding the two regions at different temperatures with a thermostatting fix, the energy added to the hot region should equal the energy subtracted from the cold region and be proportional to the heat flux moving between the regions. See the paper by Ikeshoji and Hafskjold for details of this idea. Note that thermostatting fixes such as fix nvt, fix langevin, and fix temp/rescale store the cumulative energy they add/subtract. Alternatively, the fix heat command can used in place of thermostats on each of two regions, and the resulting temperatures of the two regions monitored with the "compute temp/region" command or the temperature profile of the intermediate region monitored with the fix ave/spatial and compute ke/atom commands.

The second method is to perform a reverse non-equilibrium MD simulation using the fix thermal/conductivity command which implements the rNEMD algorithm of Muller-Platthe. Kinetic energy is swapped between atoms in two different layers of the simulation box. This induces a temperature gradient between the two layers which can be monitored with the fix ave/spatial and compute ke/atom commands. The fix tallies the cumulative energy transfer that it performs. See the fix thermal/conductivity command for details.

The third method is based on the Green-Kubo (GK) formula which relates the ensemble average of the auto-correlation of the heat flux to kappa. The heat flux can be calculated from the fluctuations of per-atom potential and kinetic energies and per-atom stress tensor in a steady-state equilibrated simulation. This is in contrast to the two preceding non-equilibrium methods, where energy flows continuously between hot and cold regions of the simulation box.

The compute heat/flux command can calculate the needed heat flux and describes how to implement the Green_Kubo formalism using additional LAMMPS commands, such as the fix ave/correlate command to calculate the needed auto-correlation. See the doc page for the compute heat/flux command for an example input script that calculates the thermal conductivity of solid Ar via the GK formalism.
6.21 Calculating viscosity

The shear viscosity \( \eta \) of a fluid can be measured in at least 3 ways using various options in LAMMPS. (See this section of the manual for an analogous discussion for thermal conductivity). \( \eta \) is a measure of the propensity of a fluid to transmit momentum in a direction perpendicular to the direction of velocity or momentum flow. Alternatively it is the resistance the fluid has to being sheared. It is given by

\[
J = -\eta \text{grad}(V_{\text{stream}})
\]

where \( J \) is the momentum flux in units of momentum per area per time. and \( \text{grad}(V_{\text{stream}}) \) is the spatial gradient of the velocity of the fluid moving in another direction, normal to the area through which the momentum flows. Viscosity thus has units of pressure-time.

The first method is to perform a non-equilibrium MD (NEMD) simulation by shearing the simulation box via the fix deform command, and using the fix nvt/sllod command to thermostat the fluid via the SLLOD equations of motion. The velocity profile setup in the fluid by this procedure can be monitored by the fix ave/spatial command, which determines \( \text{grad}(V_{\text{stream}}) \) in the equation above. E.g. the derivative in the y-direction of the \( V_x \) component of fluid motion or \( \text{grad}(V_{\text{stream}}) = dV_x/dy \). In this case, the \( \text{Pxy} \) off-diagonal component of the pressure or stress tensor, as calculated by the compute pressure command, can also be monitored, which is the \( J \) term in the equation above. See this section of the manual for details on NEMD simulations.

The second method is to perform a reverse non-equilibrium MD simulation using the fix viscosity command which implements the rNEMD algorithm of Muller-Plathe. Momentum in one dimension is swapped between atoms in two different layers of the simulation box in a different dimension. This induces a velocity gradient which can be monitored with the fix ave/spatial command. The fix tallies the cumulative momentum transfer that it performs. See the fix viscosity command for details.

The third method is based on the Green-Kubo (GK) formula which relates the ensemble average of the auto-correlation of the stress/pressure tensor to \( \eta \). This can be done in a steady-state equilibrated simulation which is in contrast to the two preceding non-equilibrium methods, where momentum flows continuously through the simulation box.

Here is an example input script that calculates the viscosity of liquid Ar via the GK formalism:

```plaintext
# Sample LAMMPS input script for viscosity of liquid Ar

units       real
variable    T equal 86.4956
variable    V equal vol
variable    dt equal 4.0
variable    p equal 400     # correlation length
variable    s equal 5       # sample interval
variable    d equal $p*$s   # dump interval

# convert from LAMMPS real units to SI
variable    kB equal 1.3806504e-23    # [J/K/ Boltzmann
variable    atm2Pa equal 101325.0
variable    A2m equal 1.0e-10
variable    fs2s equal 1.0e-15
variable    convert equal ${atm2Pa}*${atm2Pa}*${fs2s}*${A2m}*${A2m}*${A2m}

# setup problem

dimension    3
boundary     p p p
```
lattice fcc 5.376 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region box block 0 4 0 4 0 4
create_box 1 box
create_atoms 1 box
mass 1 39.948
pair_style lj/cut 13.0
pair_coeff * * 0.2381 3.405
timestep ${dt}
thermo $d

# equilibration and thermalization
velocity all create $T 102486 mom yes rot yes dist gaussian
fix NVT all nvt temp $T $T 10 drag 0.2
run 8000

# viscosity calculation, switch to NVE if desired
#unfix NVT
#fix NVE all nve
reset_timestep 0
variable pxy equal pxy
variable pxz equal pxz
variable pyz equal pyz
fix SS all ave/correlate $s $p $d &
v_pxy v_pxz v_pyz type auto file S0St.dat ave running
variable scale equal ${convert}/(${kB}*$T)*$V*$s*$dt
variable v11 equal trap(f_SS[3])/$scale
variable v22 equal trap(f_SS[4]/$scale
variable v33 equal trap(f_SS[5]/$scale
thermo_style custom step temp press v_pxy v_pxz v_pyz v_v11 v_v22 v_v33
run 100000
variable v equal (v_v11+v_v22+v_v33)/3.0
variable ndens equal count(all)/vol
print "average viscosity: $v [Pa.s/ @ $T K, $ndens /A^3"


(Horn) Horn, Swope, Pitera, Madura, Dick, Hura, and Head-Gordon, J Chem Phys, 120, 9665 (2004).

(Ikeshoji) Ikeshoji and Hafskjold, Molecular Physics, 81, 251-261 (1994).


7. Example problems

The LAMMPS distribution includes an examples sub-directory with several sample problems. Each problem is in a sub-directory of its own. Most are 2d models so that they run quickly, requiring at most a couple of minutes to run on a desktop machine. Each problem has an input script (in.*) and produces a log file (log.*) and dump file (dump.*) when it runs. Some use a data file (data.*) of initial coordinates as additional input. A few sample log file outputs on different machines and different numbers of processors are included in the directories to compare your answers to. E.g. a log file like log.crack.foo.P means it ran on P processors of machine "foo".

The dump files produced by the example runs can be animated using the xmovie tool described in the Additional Tools section of the LAMMPS documentation. Animations of many of these examples can be viewed on the Movies section of the LAMMPS WWW Site.

These are the sample problems in the examples sub-directories:

<table>
<thead>
<tr>
<th>colloid</th>
<th>big colloid particles in a small particle solvent, 2d system</th>
</tr>
</thead>
<tbody>
<tr>
<td>comb</td>
<td>models using the COMB potential</td>
</tr>
<tr>
<td>crack</td>
<td>crack propagation in a 2d solid</td>
</tr>
<tr>
<td>dipole</td>
<td>point dipolar particles, 2d system</td>
</tr>
<tr>
<td>eim</td>
<td>NaCl using the EIM potential</td>
</tr>
<tr>
<td>ellipse</td>
<td>ellipsoidal particles in spherical solvent, 2d system</td>
</tr>
<tr>
<td>flow</td>
<td>Couette and Poiseuille flow in a 2d channel</td>
</tr>
<tr>
<td>friction</td>
<td>frictional contact of spherical asperities between 2d surfaces</td>
</tr>
<tr>
<td>indent</td>
<td>spherical indenter into a 2d solid</td>
</tr>
<tr>
<td>meam</td>
<td>MEAM test for SiC and shear (same as shear examples)</td>
</tr>
<tr>
<td>melt</td>
<td>rapid melt of 3d LJ system</td>
</tr>
<tr>
<td>micelle</td>
<td>self-assembly of small lipid-like molecules into 2d bilayers</td>
</tr>
<tr>
<td>min</td>
<td>energy minimization of 2d LJ melt</td>
</tr>
<tr>
<td>msst</td>
<td>MSST shock dynamics</td>
</tr>
<tr>
<td>neb</td>
<td>nudged elastic band (NEB) calculation for barrier finding</td>
</tr>
<tr>
<td>nemd</td>
<td>non-equilibrium MD of 2d sheared system</td>
</tr>
<tr>
<td>obstacle</td>
<td>flow around two voids in a 2d channel</td>
</tr>
<tr>
<td>peptide</td>
<td>dynamics of a small solvated peptide chain (5-mer)</td>
</tr>
<tr>
<td>peri</td>
<td>Peridynamic model of cylinder impacted by indenter</td>
</tr>
<tr>
<td>pour</td>
<td>pouring of granular particles into a 3d box, then chute flow</td>
</tr>
<tr>
<td>prd</td>
<td>parallel replica dynamics of a vacancy diffusion in bulk Si</td>
</tr>
<tr>
<td>reax</td>
<td>RDX and TATB models using the ReaxFF</td>
</tr>
<tr>
<td>rigid</td>
<td>rigid bodies modeled as independent or coupled</td>
</tr>
<tr>
<td>shear</td>
<td>sideways shear applied to 2d solid, with and without a void</td>
</tr>
<tr>
<td>srd</td>
<td>stochastic rotation dynamics (SRD) particles as solvent</td>
</tr>
</tbody>
</table>

Here is how you might run and visualize one of the sample problems:

```
cd indent
cp ../src/lmp_linux .           # copy LAMMPS executable to this dir
lmp_linux <in.indent            # run the problem
```
Running the simulation produces the files *dump.indent* and *log.lammps*. You can visualize the dump file as follows:

```
../../tools/xmovie/xmovie -scale dump.indent
```

There is also an ELASTIC directory with an example script for computing elastic constants, using a zero temperature Si example. See the in.elastic file for more info.

There is also a USER directory which contains subdirectories of user-provided examples for user packages. See the README files in those directories for more info. See the doc/Section_start.html file for more info about user packages.
8. Performance & scalability

LAMMPS performance on several prototypical benchmarks and machines is discussed on the Benchmarks page of the LAMMPS WWW Site where CPU timings and parallel efficiencies are listed. Here, the benchmarks are described briefly and some useful rules of thumb about their performance are highlighted.

These are the 5 benchmark problems:

1. LJ = atomic fluid, Lennard-Jones potential with 2.5 sigma cutoff (55 neighbors per atom), NVE integration
2. Chain = bead-spring polymer melt of 100-mer chains, FENE bonds and LJ pairwise interactions with a $2^{(1/6)}$ sigma cutoff (5 neighbors per atom), NVE integration
3. EAM = metallic solid, Cu EAM potential with 4.95 Angstrom cutoff (45 neighbors per atom), NVE integration
4. Chute = granular chute flow, frictional history potential with 1.1 sigma cutoff (7 neighbors per atom), NVE integration
5. Rhodo = rhodopsin protein in solvated lipid bilayer, CHARMM force field with a 10 Angstrom LJ cutoff (440 neighbors per atom), particle-particle particle-mesh (PPPM) for long-range Coulombics, NPT integration

The input files for running the benchmarks are included in the LAMMPS distribution, as are sample output files. Each of the 5 problems has 32,000 atoms and runs for 100 timesteps. Each can be run as a serial benchmarks (on one processor) or in parallel. In parallel, each benchmark can be run as a fixed-size or scaled-size problem. For fixed-size benchmarking, the same 32K atom problem is run on various numbers of processors. For scaled-size benchmarking, the model size is increased with the number of processors. E.g. on 8 processors, a 256K-atom problem is run; on 1024 processors, a 32-million atom problem is run, etc.

A useful metric from the benchmarks is the CPU cost per atom per timestep. Since LAMMPS performance scales roughly linearly with problem size and timesteps, the run time of any problem using the same model (atom style, force field, cutoff, etc) can then be estimated. For example, on a 1.7 GHz Pentium desktop machine (Intel icc compiler under Red Hat Linux), the CPU run-time in seconds/atom/timestep for the 5 problems is

<table>
<thead>
<tr>
<th>Problem</th>
<th>LJ</th>
<th>Chain</th>
<th>EAM</th>
<th>Chute</th>
<th>Rhodopsin</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU/atom/step</td>
<td>4.55E-6</td>
<td>2.18E-6</td>
<td>9.38E-6</td>
<td>2.18E-6</td>
<td>1.11E-4</td>
</tr>
<tr>
<td>Ratio to LJ</td>
<td>1.0</td>
<td>0.48</td>
<td>2.06</td>
<td>0.48</td>
<td>24.5</td>
</tr>
</tbody>
</table>

The ratios mean that if the atomic LJ system has a normalized cost of 1.0, the bead-spring chains and granular systems run 2x faster, while the EAM metal and solvated protein models run 2x and 25x slower respectively. The bulk of these cost differences is due to the expense of computing a particular pairwise force field for a given number of neighbors per atom.

Performance on a parallel machine can also be predicted from the one-processor timings if the parallel efficiency can be estimated. The communication bandwidth and latency of a particular parallel machine affects the efficiency. On most machines LAMMPS will give fixed-size parallel efficiencies on these benchmarks above 50% so long as the atoms/processor count is a few 100 or greater - i.e. on 64 to 128 processors. Likewise, scaled-size parallel efficiencies will typically be 80% or greater up to very large processor counts. The benchmark data on the LAMMPS WWW Site gives specific examples on some different machines, including a run of 3/4 of a billion LJ atoms on 1500 processors that ran at 85% parallel efficiency.
9. Additional tools

LAMMPS is designed to be a computational kernel for performing molecular dynamics computations. Additional pre- and post-processing steps are often necessary to setup and analyze a simulation. A few additional tools are provided with the LAMMPS distribution and are described in this section.

Our group has also written and released a separate toolkit called Pizza.py which provides tools for doing setup, analysis, plotting, and visualization for LAMMPS simulations. Pizza.py is written in Python and is available for download from the Pizza.py WWW site.

Note that many users write their own setup or analysis tools or use other existing codes and convert their output to a LAMMPS input format or vice versa. The tools listed here are included in the LAMMPS distribution as examples of auxiliary tools. Some of them are not actively supported by Sandia, as they were contributed by LAMMPS users. If you have problems using them, we can direct you to the authors.

The source code for each of these codes is in the tools sub-directory of the LAMMPS distribution. There is a Makefile (which you may need to edit for your platform) which will build several of the tools which reside in that directory. Some of them are larger packages in their own sub-directories with their own Makefiles.

- amber2lmp
- binary2txt
- ch2lmp
- chain
- createatoms
- data2xmovie
- eam database
- eam generate
- eff
- emacs
- ipp
- lmp2arc
- lmp2cfg
- lmp2vmd
- matlab
- micelle2d
- msi2lmp
- pymol_asphere
- python
- reax
- restart2data
- thermo_extract
- vim
- xmovie

**amber2lmp tool**

The amber2lmp sub-directory contains two Python scripts for converting files back-and-forth between the AMBER MD code and LAMMPS. See the README file in amber2lmp for more information.
These tools were written by Keir Novik while he was at Queen Mary University of London. Keir is no longer there and cannot support these tools which are out-of-date with respect to the current LAMMPS version (and maybe with respect to AMBER as well). Since we don't use these tools at Sandia, you'll need to experiment with them and make necessary modifications yourself.

**binary2txt tool**

The file binary2txt.cpp converts one or more binary LAMMPS dump file into ASCII text files. The syntax for running the tool is

```
binary2txt file1 file2 ...
```

which creates file1.txt, file2.txt, etc. This tool must be compiled on a platform that can read the binary file created by a LAMMPS run, since binary files are not compatible across all platforms.

**ch2lmp tool**

The ch2lmp sub-directory contains tools for converting files back-and-forth between the CHARMM MD code and LAMMPS.

They are intended to make it easy to use CHARMM as a builder and as a post-processor for LAMMPS. Using charmm2lammps.pl, you can convert an ensemble built in CHARMM into its LAMMPS equivalent. Using lammps2pdb.pl you can convert LAMMPS atom dumps into pdb files.

See the README file in the ch2lmp sub-directory for more information.

These tools were created by Pieter in't Veld (pjintve at sandia.gov) and Paul Crozier (pscrozi at sandia.gov) at Sandia.

**chain tool**

The file chain.f creates a LAMMPS data file containing bead-spring polymer chains and/or monomer solvent atoms. It uses a text file containing chain definition parameters as an input. The created chains and solvent atoms can strongly overlap, so LAMMPS needs to run the system initially with a "soft" pair potential to un-overlap it. The syntax for running the tool is

```
chain <def.chain > data.file
```

See the def.chain or def.chain.ab files in the tools directory for examples of definition files. This tool was used to create the system for the chain benchmark.

**createatoms tool**

The tools/createatoms directory contains a Fortran program called createAtoms.f which can generate a variety of interesting crystal structures and geometries and output the resulting list of atom coordinates in LAMMPS or other formats.

See the included Manual.pdf for details.

The tool is authored by Xiaowang Zhou (Sandia), xzhou at sandia.gov.
data2xmovie tool

The file data2xmovie.c converts a LAMMPS data file into a snapshot suitable for visualizing with the xmovie tool, as if it had been output with a dump command from LAMMPS itself. The syntax for running the tool is

```
data2xmovie options <infile > outfile
```

See the top of the data2xmovie.c file for a discussion of the options.

eam database tool

The tools/eam_database directory contains a Fortran program that will generate EAM alloy setfl potential files for any combination of 16 elements: Cu, Ag, Au, Ni, Pd, Pt, Al, Pb, Fe, Mo, Ta, W, Mg, Co, Ti, Zr. The files can then be used with the pair_style eam/alloy command.

The tool is authored by Xiaowang Zhou (Sandia), xzhou at sandia.gov, and is based on his paper:


eam generate tool

The tools/eam_generate directory contains several one-file C programs that convert an analytic formula into a tabulated embedded atom method (EAM) setfl potential file. The potentials they produce are in the potentials directory, and can be used with the pair_style eam/alloy command.

The source files and potentials were provided by Gerolf Ziegenhain (gerolf at ziegenhain.com).

eff tool

The tools/eff directory contains various scripts for generating structures and post-processing output for simulations using the electron force field (eFF).

These tools were provided by Andres Jaramillo-Botero at CalTech (ajaramil at wag.caltech.edu).

emacs tool

The tools/emacs directory contains a Lips add-on file for Emacs that enables a lammps-mode for editing of input scripts when using Emacs, with various highlighting options setup.

These tools were provided by Aidan Thompson at Sandia (athomps at sandia.gov).

ipp tool

The tools/ipp directory contains a Perl script ipp which can be used to facilitate the creation of a complicated file (say, a lammps input script or tools/createatoms input file) using a template file.

ipp was created and is maintained by Reese Jones (Sandia), rjones at sandia.gov.

See two examples in the tools/ipp directory. One of them is for the tools/createatoms tool's input file.
**lmp2arc tool**

The lmp2arc sub-directory contains a tool for converting LAMMPS output files to the format for Accelrys' Insight MD code (formerly MSI/Biosym and its Discover MD code). See the README file for more information.

This tool was written by John Carpenter (Cray), Michael Peachey (Cray), and Steve Lustig (Dupont). John is now at the Mayo Clinic (jec at mayo.edu), but still fields questions about the tool.

This tool was updated for the current LAMMPS C++ version by Jeff Greathouse at Sandia (jagreat at sandia.gov).

**lmp2cfg tool**

The lmp2cfg sub-directory contains a tool for converting LAMMPS output files into a series of *.cfg files which can be read into the AtomEye visualizer. See the README file for more information.

This tool was written by Ara Kooser at Sandia (askoose at sandia.gov).

**lmp2vmd tool**

The lmp2vmd sub-directory contains a README.txt file that describes details of scripts and plugin support within the VMD package for visualizing LAMMPS dump files.

The VMD plugins and other supporting scripts were written by Axel Kohlmeyer (akohlmey at cmm.chem.upenn.edu) at U Penn.

**matlab tool**

The matlab sub-directory contains several MATLAB scripts for post-processing LAMMPS output. The scripts include readers for log and dump files, a reader for EAM potential files, and a converter that reads LAMMPS dump files and produces CFG files that can be visualized with the AtomEye visualizer.

See the README.pdf file for more information.

These scripts were written by Arun Subramaniyan at Purdue Univ (asubrama at purdue.edu).

**micelle2d tool**

The file micelle2d.f creates a LAMMPS data file containing short lipid chains in a monomer solution. It uses a text file containing lipid definition parameters as an input. The created molecules and solvent atoms can strongly overlap, so LAMMPS needs to run the system initially with a "soft" pair potential to un-overlap it. The syntax for running the tool is

```
micelle2d <def.micelle2d > data.file
```

See the def.micelle2d file in the tools directory for an example of a definition file. This tool was used to create the system for the micelle example.

**msi2lmp tool**

The msi2lmp sub-directory contains a tool for creating LAMMPS input data files from Accelrys' Insight MD code (formerly MSI/Biosym and its Discover MD code). See the README file for more information.
This tool was written by John Carpenter (Cray), Michael Peache (Cray), and Steve Lustig (Dupont). John is now at the Mayo Clinic (jec at mayo.edu), but still fields questions about the tool.

This tool may be out-of-date with respect to the current LAMMPS and Insight versions. Since we don't use it at Sandia, you'll need to experiment with it yourself.

**pymol_asphere tool**

The pymol_asphere sub-directory contains a tool for converting a LAMMPS dump file that contains orientation info for ellipsoidal particles into an input file for the PyMol visualization package.

Specifically, the tool triangulates the ellipsoids so they can be viewed as true ellipsoidal particles within PyMol. See the README and examples directory within pymol_asphere for more information.

This tool was written by Mike Brown at Sandia.

**python tool**

The python sub-directory contains several Python scripts that perform common LAMMPS post-processing tasks, such as:

- extract thermodynamic info from a log file as columns of numbers
- plot two columns of thermodynamic info from a log file using GnuPlot
- sort the snapshots in a dump file by atom ID
- convert multiple NEB dump files into one dump file for viz
- convert dump files into XYZ, CFG, or PDB format for viz by other packages

These are simple scripts built on Pizza.py modules. See the README for more info on Pizza.py and how to use these scripts.

**reax tool**

The reax sub-directory contains stand-alond codes that can post-process the output of the fix reax/bonds command from a LAMMPS simulation using ReaxFF. See the README.txt file for more info.

These tools were written by Aidan Thompson at Sandia.

**restart2data tool**

The file restart2data.cpp converts a binary LAMMPS restart file into an ASCII data file. The syntax for running the tool is

```
restart2data restart-file data-file (input-file)
```

Input-file is optional and if specified will contain LAMMPS input commands for the masses and force field parameters, instead of putting those in the data-file. Only a few force field styles currently support this option.

This tool must be compiled on a platform that can read the binary file created by a LAMMPS run, since binary files are not compatible across all platforms.

Note that a text data file has less precision than a binary restart file. Hence, continuing a run from a converted data file will typically not conform as closely to a previous run as will restarting from a binary restart file.
If a "%" appears in the specified restart-file, the tool expects a set of multiple files to exist. See the \texttt{restart} and \texttt{write_restart} commands for info on how such sets of files are written by LAMMPS, and how the files are named.

\textbf{thermo\_extract tool}

The \texttt{thermo\_extract} tool reads one of more LAMMPS log files and extracts a thermodynamic value (e.g. Temp, Press). It spits out the time,value as 2 columns of numbers so the tool can be used as a quick way to plot some quantity of interest. See the header of the \texttt{thermo\_extract.c} file for the syntax of how to run it and other details.

This tool was written by Vikas Varshney at Wright Patterson AFB (vikas.varshney at gmail.com).

\textbf{vim tool}

The files in the tools/vim directory are add-ons to the VIM editor that allow easier editing of LAMMPS input scripts. See the \texttt{README.txt} file for details.

These files were provided by Gerolf Ziegenhain (gerolf at ziegenhain.com)

\textbf{xmovie tool}

The \texttt{xmovie} tool is an X-based visualization package that can read LAMMPS dump files and animate them. It is in its own sub-directory with the tools directory. You may need to modify its Makefile so that it can find the appropriate X libraries to link against.

The syntax for running \texttt{xmovie} is

\begin{verbatim}
xmovie \texttt{options} dump.file1 dump.file2 ...
\end{verbatim}

If you just type "\texttt{xmovie}" you will see a list of options. Note that by default, LAMMPS dump files are in scaled coordinates, so you typically need to use the -scale option with \texttt{xmovie}. When \texttt{xmovie} runs it opens a visualization window and a control window. The control options are straightforward to use.

\texttt{Xmovie} was mostly written by Mike Uttormark (U Wisconsin) while he spent a summer at Sandia. It displays 2d projections of a 3d domain. While simple in design, it is an amazingly fast program that can render large numbers of atoms very quickly. It's a useful tool for debugging LAMMPS input and output and making sure your simulation is doing what you think it should. The animations on the Examples page of the LAMMPS WWW site were created with \texttt{xmovie}.

I've lost contact with Mike, so I hope he's comfortable with us distributing his great tool!
10. Modifying & extending LAMMPS

This section describes how to customize LAMMPS by modifying and extending its source code.

10.1 Atom styles
10.2 Bond, angle, dihedral, improper potentials
10.3 Compute styles
10.4 Dump styles
10.5 Dump custom output options
10.6 Fix styles which include integrators, temperature and pressure control, force constraints, boundary conditions, diagnostic output, etc
10.7 Input script commands
10.8 Kspace computations
10.9 Minimization styles
10.10 Pairwise potentials
10.11 Region styles
10.12 Thermodynamic output options
10.13 Variable options
10.14 Submitting new features for inclusion in LAMMPS

LAMMPS is designed in a modular fashion so as to be easy to modify and extend with new functionality. In fact, about 75% of its source code is files added in this fashion.

In this section, changes and additions users can make are listed along with minimal instructions. If you add a new feature to LAMMPS and think it will be of interest to general users, we encourage you to submit it to the developers for inclusion in the released version of LAMMPS. Information about how to do this is provided below.

The best way to add a new feature is to find a similar feature in LAMMPS and look at the corresponding source and header files to figure out what it does. You will need some knowledge of C++ to be able to understand the hi-level structure of LAMMPS and its class organization, but functions (class methods) that do actual computations are written in vanilla C-style code and operate on simple C-style data structures (vectors and arrays).

Most of the new features described in this section require you to write a new C++ derived class (except for exceptions described below, where you can make small edits to existing files). Creating a new class requires 2 files, a source code file (*.cpp) and a header file (*.h). The derived class must provide certain methods to work as a new option. Depending on how different your new feature is compared to existing features, you can either derive from the base class itself, or from a derived class that already exists. Enabling LAMMPS to invoke the new class is as simple as putting the two source files in the src dir and re-building LAMMPS.

The advantage of C++ and its object-orientation is that all the code and variables needed to define the new feature are in the 2 files you write, and thus shouldn't make the rest of LAMMPS more complex or cause side-effect bugs.

Here is a concrete example. Suppose you write 2 files pair_foo.cpp and pair_foo.h that define a new class PairFoo that computes pairwise potentials described in the classic 1997 paper by Foo, et al. If you wish to invoke those potentials in a LAMMPS input script with a command like

```
pair_style foo 0.1 3.5
```

then your pair_foo.h file should be structured as follows:
where "foo" is the style keyword in the pair_style command, and PairFoo is the class name defined in your pair_foo.cpp and pair_foo.h files.

When you re-build LAMMPS, your new pairwise potential becomes part of the executable and can be invoked with a pair_style command like the example above. Arguments like 0.1 and 3.5 can be defined and processed by your new class.

As illustrated by this pairwise example, many kinds of options are referred to in the LAMMPS documentation as the "style" of a particular command.

The instructions below give the header file for the base class that these styles are derived from. Public variables in that file are ones used and set by the derived classes which are also used by the base class. Sometimes they are also used by the rest of LAMMPS. Virtual functions in the base class header file which are set = 0 are ones you must define in your new derived class to give it the functionality LAMMPS expects. Virtual functions that are not set to 0 are functions you can optionally define.

Additionally, new output options can be added directly to the thermo.cpp, dump_custom.cpp, and variable.cpp files as explained below.

Here are additional guidelines for modifying LAMMPS and adding new functionality:

- Think about whether what you want to do would be better as a pre- or post-processing step. Many computations are more easily and more quickly done that way.
- Don't do anything within the timestepping of a run that isn't parallel. E.g. don't accumulate a bunch of data on a single processor and analyze it. You run the risk of seriously degrading the parallel efficiency.
- If your new feature reads arguments or writes output, make sure you follow the unit conventions discussed by the units command.
- If you add something you think is truly useful and doesn't impact LAMMPS performance when it isn't used, send an email to the developers. We might be interested in adding it to the LAMMPS distribution. See further details on this at the bottom of this page.

10.1 Atom styles

Classes that define an atom style are derived from the AtomVec class and managed by the Atom class. The atom style determines what quantities are associated with an atom. A new atom style can be created if one of the existing atom styles does not define all the arrays you need to store and communicate with atoms.

Atom_vec_atomic.cpp is a simple example of an atom style.

Here is a brief description of methods you define in your new derived class. See atom_vec.h for details.

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>init</td>
<td>one time setup (optional)</td>
</tr>
<tr>
<td>grow</td>
<td>re-allocate atom arrays to longer lengths (required)</td>
</tr>
</tbody>
</table>
grow_reset  make array pointers in Atom and AtomVec classes consistent (required)
copy      copy info for one atom to another atom's array locations (required)
pack_comm store an atom's info in a buffer communicated every timestep (required)
pack_comm_vel add velocity info to communication buffer (required)
pack_comm_hybrid store extra info unique to this atom style (optional)
unpack_comm retrieve an atom's info from the buffer (required)
unpack_comm_vel also retrieve velocity info (required)
unpack_comm_hybrid retrieve extra info unique to this atom style (optional)
pack_reverse store an atom's info in a buffer communicating partial forces (required)
pack_reverse_hybrid store extra info unique to this atom style (optional)
unpack_reverse retrieve an atom's info from the buffer (required)
unpack_reverse_hybrid retrieve extra info unique to this atom style (optional)
pack_border store an atom's info in a buffer communicated on neighbor re-builds (required)
pack_border_vel add velocity info to buffer (required)
pack_border_hybrid store extra info unique to this atom style (optional)
unpack_border retrieve an atom's info from the buffer (required)
unpack_border_vel also retrieve velocity info (required)
unpack_border_hybrid retrieve extra info unique to this atom style (optional)
pack_exchange store all an atom's info to migrate to another processor (required)
unpack_exchange retrieve an atom's info from the buffer (required)
size_restart number of restart quantities associated with proc's atoms (required)
pack_restart pack atom quantities into a buffer (required)
unpack_restart unpack atom quantities from a buffer (required)
create_atom create an individual atom of this style (required)
data_atom parse an atom line from the data file (required)
data_atom_hybrid parse additional atom info unique to this atom style (optional)
data_vel parse one line of velocity information from data file (optional)
data_vel_hybrid parse additional velocity data unique to this atom style (optional)
memory_usage tally memory allocated by atom arrays (required)

The constructor of the derived class sets values for several variables that you must set when defining a new atom style, which are documented in atom_vec.h. New atom arrays are defined in atom.cpp. Search for the word "customize" and you will find locations you will need to modify.

10.2 Bond, angle, dihedral, improper potentials

Classes that compute molecular interactions are derived from the Bond, Angle, Dihedral, and Improper classes. New styles can be created to add new potentials to LAMMPS.

Bond_harmonic.cpp is the simplest example of a bond style. Ditto for the harmonic forms of the angle, dihedral, and improper style commands.

Here is a brief description of common methods you define in your new derived class. See bond.h, angle.h, dihedral.h, and improper.h for details and specific additional methods.
10.3 Compute styles

Classes that compute scalar and vector quantities like temperature and the pressure tensor, as well as classes that compute per-atom quantities like kinetic energy and the centro-symmetry parameter are derived from the Compute class. New styles can be created to add new calculations to LAMMPS.

Compute_temp.cpp is a simple example of computing a scalar temperature. Compute_ke_atom.cpp is a simple example of computing per-atom kinetic energy.

Here is a brief description of methods you define in your new derived class. See compute.h for details.

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>init</td>
<td>perform one time setup (required)</td>
</tr>
<tr>
<td>init_list</td>
<td>neighbor list setup, if needed (optional)</td>
</tr>
<tr>
<td>compute_scalar</td>
<td>compute a scalar quantity (optional)</td>
</tr>
<tr>
<td>compute_vector</td>
<td>compute a vector of quantities (optional)</td>
</tr>
<tr>
<td>compute_peratom</td>
<td>compute one or more quantities per atom (optional)</td>
</tr>
<tr>
<td>compute_local</td>
<td>compute one or more quantities per processor (optional)</td>
</tr>
<tr>
<td>pack_comm</td>
<td>pack a buffer with items to communicate (optional)</td>
</tr>
<tr>
<td>unpack_comm</td>
<td>unpack the buffer (optional)</td>
</tr>
<tr>
<td>pack_reverse</td>
<td>pack a buffer with items to reverse communicate (optional)</td>
</tr>
<tr>
<td>unpack_reverse</td>
<td>unpack the buffer (optional)</td>
</tr>
<tr>
<td>remove_bias</td>
<td>remove velocity bias from one atom (optional)</td>
</tr>
<tr>
<td>remove_bias_all</td>
<td>remove velocity bias from all atoms in group (optional)</td>
</tr>
<tr>
<td>restore_bias</td>
<td>restore velocity bias for one atom after remove_bias (optional)</td>
</tr>
<tr>
<td>restore_bias_all</td>
<td>same as before, but for all atoms in group (optional)</td>
</tr>
<tr>
<td>memory_usage</td>
<td>tally memory usage (optional)</td>
</tr>
</tbody>
</table>

10.4 Dump styles
10.5 Dump custom output options

Classes that dump per-atom info to files are derived from the Dump class. To dump new quantities or in a new format, a new derived dump class can be added, but it is typically simpler to modify the DumpCustom class contained in the dump_custom.cpp file.

Dump_atom.cpp is a simple example of a derived dump class.

Here is a brief description of methods you define in your new derived class. See dump.h for details.

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>write_header</td>
<td>write the header section of a snapshot of atoms</td>
</tr>
<tr>
<td>count</td>
<td>count the number of lines a processor will output</td>
</tr>
<tr>
<td>pack</td>
<td>pack a proc's output data into a buffer</td>
</tr>
<tr>
<td>write_data</td>
<td>write a proc's data to a file</td>
</tr>
</tbody>
</table>

See the dump command and its custom style for a list of keywords for atom information that can already be dumped by DumpCustom. It includes options to dump per-atom info from Compute classes, so adding a new derived Compute class is one way to calculate new quantities to dump.

Alternatively, you can add new keywords to the dump custom command. Search for the word "customize" in dump_custom.cpp to see the half-dozen or so locations where code will need to be added.

10.6 Fix styles

In LAMMPS, a "fix" is any operation that is computed during timestepping that alters some property of the system. Essentially everything that happens during a simulation besides force computation, neighbor list construction, and output, is a "fix". This includes time integration (update of coordinates and velocities), force constraints or boundary conditions (SHAKE or walls), and diagnostics (compute a diffusion coefficient). New styles can be created to add new options to LAMMPS.

Fix_setforce.cpp is a simple example of setting forces on atoms to prescribed values. There are dozens of fix options already in LAMMPS; choose one as a template that is similar to what you want to implement.

Here is a brief description of methods you can define in your new derived class. See fix.h for details.

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>setmask</td>
<td>determines when the fix is called during the timestep (required)</td>
</tr>
<tr>
<td>init</td>
<td>initialization before a run (optional)</td>
</tr>
<tr>
<td>setup_pre_exchange</td>
<td>called before atom exchange in setup (optional)</td>
</tr>
<tr>
<td>setup_pre_force</td>
<td>called before force computation in setup (optional)</td>
</tr>
<tr>
<td>setup</td>
<td>called immediately before the 1st timestep and after forces are computed (optional)</td>
</tr>
<tr>
<td>min_setup_pre_force</td>
<td>like setup_pre_force, but for minimizations instead of MD runs (optional)</td>
</tr>
<tr>
<td>min_setup</td>
<td>like setup, but for minimizations instead of MD runs (optional)</td>
</tr>
<tr>
<td>initial_integrate</td>
<td>called at very beginning of each timestep (optional)</td>
</tr>
<tr>
<td>pre_exchange</td>
<td>called before atom exchange on re-neighboring steps (optional)</td>
</tr>
<tr>
<td>pre_neighbor</td>
<td>called before neighbor list build (optional)</td>
</tr>
<tr>
<td>pre_force</td>
<td>called after pair &amp; molecular forces are computed (optional)</td>
</tr>
<tr>
<td>post_force</td>
<td>called after pair &amp; molecular forces are computed and communicated (optional)</td>
</tr>
<tr>
<td>final_integrate</td>
<td>called at end of each timestep (optional)</td>
</tr>
<tr>
<td>Method</td>
<td>Description</td>
</tr>
<tr>
<td>-----------------------------</td>
<td>------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>end_of_step</td>
<td>called at very end of timestep (optional)</td>
</tr>
<tr>
<td>write_restart</td>
<td>dumps fix info to restart file (optional)</td>
</tr>
<tr>
<td>restart</td>
<td>uses info from restart file to re-initialize the fix (optional)</td>
</tr>
<tr>
<td>grow_arrays</td>
<td>allocate memory for atom-based arrays used by fix (optional)</td>
</tr>
<tr>
<td>copy_arrays</td>
<td>copy atom info when an atom migrates to a new processor (optional)</td>
</tr>
<tr>
<td>pack_exchange</td>
<td>store atom's data in a buffer (optional)</td>
</tr>
<tr>
<td>unpack_exchange</td>
<td>retrieve atom's data from a buffer (optional)</td>
</tr>
<tr>
<td>pack_restart</td>
<td>store atom's data for writing to restart file (optional)</td>
</tr>
<tr>
<td>unpack_restart</td>
<td>retrieve atom's data from a restart file buffer (optional)</td>
</tr>
<tr>
<td>size_restart</td>
<td>size of atom's data (optional)</td>
</tr>
<tr>
<td>maxsize_restart</td>
<td>max size of atom's data (optional)</td>
</tr>
<tr>
<td>setup_pre_force_respa</td>
<td>same as setup_pre_force, but for rRESPA (optional)</td>
</tr>
<tr>
<td>initial_integrate_respa</td>
<td>same as initial_integrate, but for rRESPA (optional)</td>
</tr>
<tr>
<td>post_integrate_respa</td>
<td>called after the first half integration step is done in rRESPA (optional)</td>
</tr>
<tr>
<td>pre_force_respa</td>
<td>same as pre_force, but for rRESPA (optional)</td>
</tr>
<tr>
<td>post_force_respa</td>
<td>same as post_force, but for rRESPA (optional)</td>
</tr>
<tr>
<td>final_integrate_respa</td>
<td>same as final_integrate, but for rRESPA (optional)</td>
</tr>
<tr>
<td>min_pre_force</td>
<td>called after pair &amp; molecular forces are computed in minimizer (optional)</td>
</tr>
<tr>
<td>min_post_force</td>
<td>called after pair &amp; molecular forces are computed and communicated in minimizer (optional)</td>
</tr>
<tr>
<td>min_store</td>
<td>store extra data for linesearch based minimization on a LIFO stack (optional)</td>
</tr>
<tr>
<td>min_pushstore</td>
<td>push the minimization LIFO stack one element down (optional)</td>
</tr>
<tr>
<td>min_popstore</td>
<td>pop the minimization LIFO stack one element up (optional)</td>
</tr>
<tr>
<td>min_clearstore</td>
<td>clear minimization LIFO stack (optional)</td>
</tr>
<tr>
<td>min_step</td>
<td>reset or move forward on line search minimization (optional)</td>
</tr>
<tr>
<td>min_dof</td>
<td>report number of degrees of freedom added by this fix in minimization (optional)</td>
</tr>
<tr>
<td>max_alpha</td>
<td>report maximum allowed step size during linesearch minimization (optional)</td>
</tr>
<tr>
<td>pack_comm</td>
<td>pack a buffer to communicate a per-atom quantity (optional)</td>
</tr>
<tr>
<td>unpack_comm</td>
<td>unpack a buffer to communicate a per-atom quantity (optional)</td>
</tr>
<tr>
<td>pack_reverse_comm</td>
<td>pack a buffer to reverse communicate a per-atom quantity (optional)</td>
</tr>
<tr>
<td>unpack_reverse_comm</td>
<td>unpack a buffer to reverse communicate a per-atom quantity (optional)</td>
</tr>
<tr>
<td>dof</td>
<td>report number of degrees of freedom removed by this fix during MD (optional)</td>
</tr>
<tr>
<td>compute_scalar</td>
<td>return a global scalar property that the fix computes (optional)</td>
</tr>
<tr>
<td>compute_vector</td>
<td>return a component of a vector property that the fix computes (optional)</td>
</tr>
<tr>
<td>compute_array</td>
<td>return a component of an array property that the fix computes (optional)</td>
</tr>
<tr>
<td>deform</td>
<td>called when the box size is changed (optional)</td>
</tr>
<tr>
<td>reset_target</td>
<td>called when a change of the target temperature is requested during a run (optional)</td>
</tr>
<tr>
<td>reset_dt</td>
<td>is called when a change of the time step is requested during a run (optional)</td>
</tr>
<tr>
<td>modify_param</td>
<td>called when a fix_modify request is executed (optional)</td>
</tr>
<tr>
<td>memory_usage</td>
<td>report memory used by fix (optional)</td>
</tr>
<tr>
<td>thermo</td>
<td>compute quantities for thermodynamic output (optional)</td>
</tr>
</tbody>
</table>

Typically, only a small fraction of these methods are defined for a particular fix. Setmask is mandatory, as it determines when the fix will be invoked during the timestep. Fixes that perform time integration (nve, nvt, npt)
implement initial_integrate() and final_integrate() to perform velocity Verlet updates. Fixes that constrain forces implement post_force().

Fixes that perform diagnostics typically implement end_of_step(). For an end_of_step fix, one of your fix arguments must be the variable "nevery" which is used to determine when to call the fix and you must set this variable in the constructor of your fix. By convention, this is the first argument the fix defines (after the ID, group-ID, style).

If the fix needs to store information for each atom that persists from timestep to timestep, it can manage that memory and migrate the info with the atoms as they move from processors to processor by implementing the grow_arrays, copy_arrays, pack_exchange, and unpack_exchange methods. Similarly, the pack_restart and unpack_restart methods can be implemented to store information about the fix in restart files. If you wish an integrator or force constraint fix to work with rRESPA (see the run_style command), the initial_integrate, post_force_integrate, and final_integrate_respa methods can be implemented. The thermo method enables a fix to contribute values to thermodynamic output, as printed quantities and/or to be summed to the potential energy of the system.

10.7 Input script commands

New commands can be added to LAMMPS input scripts by adding new classes that have a "command" method. For example, the create_atoms, read_data, velocity, and run commands are all implemented in this fashion. When such a command is encountered in the LAMMPS input script, LAMMPS simply creates a class with the corresponding name, invokes the "command" method of the class, and passes it the arguments from the input script. The command method can perform whatever operations it wishes on LAMMPS data structures.

The single method your new class must define is as follows:

| command | operations performed by the new command |

Of course, the new class can define other methods and variables as needed.

10.8 Kspace computations

Classes that compute long-range Coulombic interactions via K-space representations (Ewald, PPPM) are derived from the KSpace class. New styles can be created to add new K-space options to LAMMPS.

Ewald.cpp is an example of computing K-space interactions.

Here is a brief description of methods you define in your new derived class. See kspace.h for details.

| init     | initialize the calculation before a run |
| setup    | computation before the 1st timestep of a run |
| compute  | every-timestep computation |
| memory_usage | tally of memory usage |

10.9 Minimization styles

Classes that perform energy minimization derived from the Min class. New styles can be created to add new minimization algorithms to LAMMPS.
Min_cg.cpp is an example of conjugate gradient minimization.

Here is a brief description of methods you define in your new derived class. See min.h for details.

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>init</td>
<td>initialize the minimization before a run</td>
</tr>
<tr>
<td>run</td>
<td>perform the minimization</td>
</tr>
<tr>
<td>memory_usage</td>
<td>tally of memory usage</td>
</tr>
</tbody>
</table>

10.10 Pairwise potentials

Classes that compute pairwise interactions are derived from the Pair class. In LAMMPS, pairwise calculation include manybody potentials such as EAM or Tersoff where particles interact without a static bond topology. New styles can be created to add new pair potentials to LAMMPS.

Pair_lj_cut.cpp is a simple example of a Pair class, though it includes some optional methods to enable its use with rRESPA.

Here is a brief description of the class methods in pair.h:

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>compute</td>
<td>workhorse routine that computes pairwise interactions</td>
</tr>
<tr>
<td>settings</td>
<td>reads the input script line with arguments you define</td>
</tr>
<tr>
<td>coeff</td>
<td>set coefficients for one i,j type pair</td>
</tr>
<tr>
<td>init_one</td>
<td>perform initialization for one i,j type pair</td>
</tr>
<tr>
<td>init_style</td>
<td>initialization specific to this pair style</td>
</tr>
<tr>
<td>write &amp; read_restart</td>
<td>write/read i,j pair coeffs to restart files</td>
</tr>
<tr>
<td>write &amp; read_restart_settings</td>
<td>write/read global settings to restart files</td>
</tr>
<tr>
<td>single</td>
<td>force and energy of a single pairwise interaction between 2 atoms</td>
</tr>
<tr>
<td>compute_inner/middle/outer</td>
<td>versions of compute used by rRESPA</td>
</tr>
</tbody>
</table>

The inner/middle/outer routines are optional.

10.11 Region styles

Classes that define geometric regions are derived from the Region class. Regions are used elsewhere in LAMMPS to group atoms, delete atoms to create a void, insert atoms in a specified region, etc. New styles can be created to add new region shapes to LAMMPS.

Region_sphere.cpp is an example of a spherical region.

Here is a brief description of methods you define in your new derived class. See region.h for details.

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>match</td>
<td>determine whether a point is in the region</td>
</tr>
</tbody>
</table>
10.12 Thermodynamic output options

There is one class that computes and prints thermodynamic information to the screen and log file; see the file thermo.cpp.

There are two styles defined in thermo.cpp: "one" and "multi". There is also a flexible "custom" style which allows the user to explicitly list keywords for quantities to print when thermodynamic info is output. See the thermo_style command for a list of defined quantities.

The thermo styles (one, multi, etc) are simply lists of keywords. Adding a new style thus only requires defining a new list of keywords. Search for the word "customize" with references to "thermo style" in thermo.cpp to see the two locations where code will need to be added.

New keywords can also be added to thermo.cpp to compute new quantities for output. Search for the word "customize" with references to "keyword" in thermo.cpp to see the several locations where code will need to be added.

Note that the thermo_style custom command already allows for thermo output of quantities calculated by fixes, computes, and variables. Thus, it may be simpler to compute what you wish via one of those constructs, than by adding a new keyword to the thermo command.

10.13 Variable options

There is one class that computes and stores variable information in LAMMPS; see the file variable.cpp. The value associated with a variable can be periodically printed to the screen via the print, fix print, or thermo_style custom commands. Variables of style "equal" can compute complex equations that involve the following types of arguments:

thermo keywords = ke, vol, atoms, ... other variables = v_a, v_myvar, ... math functions = div(x,y), mult(x,y),
add(x,y), ... group functions = mass(group), xcm(group,x), ... atom values = x123, y3, vx34, ... compute values =
c_mytemp0, c_thermo_press3, ...

Adding keywords for the thermo_style custom command (which can then be accessed by variables) was discussed here on this page.

Adding a new math function of one or two arguments can be done by editing one section of the Variable::evaulate() method. Search for the word "customize" to find the appropriate location.

Adding a new group function can be done by editing one section of the Variable::evaulate() method. Search for the word "customize" to find the appropriate location. You may need to add a new method to the Group class as well (see the group.cpp file).

Accessing a new atom-based vector can be done by editing one section of the Variable::evaulate() method. Search for the word "customize" to find the appropriate location.

Adding new compute styles (whose calculated values can then be accessed by variables) was discussed here on this page.
10.14 Submitting new features for inclusion in LAMMPS

We encourage users to submit new features that they add to LAMMPS to the developers, especially if you think the features will be of interest to other users. If they are broadly useful we may add them as core files to LAMMPS or as part of a standard package. Else we will add them as a user-contributed package or file. Examples of user packages are in src sub-directories that start with USER. The USER-MISC package is simply a collection of (mostly) unrelated single files, which is the simplest way to have your contribution quickly added to the LAMMPS distribution. You can see a list of the both standard and user packages by typing "make package" in the LAMMPS src directory.

With user packages and files, all we are really providing (aside from the fame and fortune that accompanies having your name in the source code and on the Authors page of the LAMMPS WWW site), is a means for you to distribute your work to the LAMMPS user community and a mechanism for others to easily try out your new feature. This may help you find bugs or make contact with new collaborators. Note that you're also implicitly agreeing to support your code which means answer questions, fix bugs, and maintain it if LAMMPS changes.

The previous sections of this doc page describe how to add new features of various kinds to LAMMPS. Packages are simply collections of one or more new class files which are invoked as a new "style" within a LAMMPS input script. If designed correctly, these additions do not require changes to the main core of LAMMPS; they are simply add-on files. If you think your new feature requires non-trivial changes in core LAMMPS files, you'll need to communicate with the developers, since we may or may not want to make those changes. An example of a trivial change is making a parent-class method "virtual" when you derive a new child class from it.

Here is what you need to do to submit a user package or single file for our consideration. Following these steps will save time for both you and us. See existing package files for examples.

- All source files you provide must compile with the most current version of LAMMPS.
- If your contribution is a single file (actually a *.cpp and *.h file) it can most rapidly be added to the USER-MISC directory. Send us the one-line entry to add to the USER-MISC/README file in that dir, along with the 2 source files. You can do this multiple times if you wish to contribute several individual features.
- If your contribution is several related features, it is probably best to make it a user package directory with a name like USER-FOO. In addition to your new files, the directory should contain a README, and Install.csh file. The README text file should contain your name and contact information and a brief description of what your new package does. The Install.csh file enables LAMMPS to include and exclude your package. See other README and Install.sh files in other USER directories as examples. Send us a tarball of this USER-FOO directory.
- Your new source files need to have the LAMMPS copyright, GPL notice, and your name at the top, like other LAMMPS source files. They need to create a class that is inside the LAMMPS namespace. Other than that, your files can do whatever is necessary to implement the new features. They don't have to be written in the same stylistic format and syntax as other LAMMPS files, though that would be nice.
- Finally, you must also send a documentation file for each new command or style you are adding to LAMMPS. This will be one file for a single-file feature. For a package, it might be several files. These are simple text files which we will convert to HTML. They must be in the same format as other *.txt files in the lammps/doc directory for similar commands and styles. The "Restrictions" section of the doc page should indicate that your command is only available if LAMMPS is built with the appropriate USER-MISC or USER-FOO package. See other user package doc files for an example of how to do this. The txt2html tool we use to do the conversion can be downloaded from this site, so you can perform the HTML conversion yourself to proofread your doc page.

Note that the more clear and self-explanatory you make your doc and README files, the more likely it is that users will try out your new feature.
(Foo) Foo, Morefoo, and Maxfoo, J of Classic Potentials, 75, 345 (1997).
11. Python interface to LAMMPS

This section describes how to build and use LAMMPS via a Python interface.

- 11.1 Building LAMMPS as a shared library
- 11.2 Installing the Python wrapper into Python
- 11.3 Extending Python with MPI to run in parallel
- 11.4 Testing the Python-LAMMPS interface
- 11.5 Using LAMMPS from Python
- 11.6 Example Python scripts that use LAMMPS

The LAMMPS distribution includes the file python/lammps.py which wraps the library interface to LAMMPS. This file makes it possible to run LAMMPS, invoke LAMMPS commands or give it an input script, extract LAMMPS results, an modify internal LAMMPS variables, either from a Python script or interactively from a Python prompt. You can do the former in serial or parallel. Running Python interactively in parallel does not generally work, unless you have a package installed that extends your Python to enable multiple instances of Python to read what you type.

Python is a powerful scripting and programming language which can be used to wrap software like LAMMPS and other packages. It can be used to glue multiple pieces of software together, e.g. to run a coupled or multiscale model. See Section section of the manual and the couple directory of the distribution for more ideas about coupling LAMMPS to other codes. See Section_start 4 about how to build LAMMPS as a library, and Section_howto 19 for a description of the library interface provided in src/library.cpp and src/library.h and how to extend it for your needs. As described below, that interface is what is exposed to Python. It is designed to be easy to add functions to. This can easily extend the Python interface as well. See details below.

By using the Python interface, LAMMPS can also be coupled with a GUI or other visualization tools that display graphs or animations in real time as LAMMPS runs. Examples of such scripts are included in the python directory.

Two advantages of using Python are how concise the language is, and that it can be run interactively, enabling rapid development and debugging of programs. If you use it to mostly invoke costly operations within LAMMPS, such as running a simulation for a reasonable number of timesteps, then the overhead cost of invoking LAMMPS thru Python will be negligible.

Before using LAMMPS from a Python script, you need to do two things. You need to build LAMMPS as a dynamic shared library, so it can be loaded by Python. And you need to tell Python how to find the library and the Python wrapper file python/lammps.py. Both these steps are discussed below. If you wish to run LAMMPS in parallel from Python, you also need to extend your Python with MPI. This is also discussed below.

The Python wrapper for LAMMPS uses the amazing and magical (to me) "ctypes" package in Python, which auto-generates the interface code needed between Python and a set of C interface routines for a library. Ctypes is part of standard Python for versions 2.5 and later. You can check which version of Python you have installed, by simply typing "python" at a shell prompt.
11.1 Building LAMMPS as a shared library

Instructions on how to build LAMMPS as a shared library are given in Section 5. A shared library is one that is dynamically loadable, which is what Python requires. On Linux this is a library file that ends in ".so", not ".a".

From the src directory, type

```
make makeshlib
make -f Makefile.shlib foo
```

where foo is the machine target name, such as linux or g++ or serial. This should create the file liblammps_foo.so in the src directory, as well as a soft link liblammps.so, which is what the Python wrapper will load by default. Note that if you are building multiple machine versions of the shared library, the soft link is always set to the most recently built version.

If this fails, see Section 5 for more details, especially if your LAMMPS build uses auxiliary libraries like MPI or FFTW which may not be built as shared libraries on your system.

11.2 Installing the Python wrapper into Python

For Python to invoke LAMMPS, there are 2 files it needs to know about:

- `python/lammps.py`
- `src/liblammps.so`

Lammps.py is the Python wrapper on the LAMMPS library interface. Liblammps.so is the shared LAMMPS library that Python loads, as described above.

You can insure Python can find these files in one of two ways:

- set two environment variables
- run the python/install.py script

If you set the paths to these files as environment variables, you only have to do it once. For the csh or tcsh shells, add something like this to your ~/.cshrc file, one line for each of the two files:

```
setenv PYTHONPATH $PYTHONPATH:/home/sjplimp/lammps/python
setenv LD_LIBRARY_PATH $LD_LIBRARY_PATH:/home/sjplimp/lammps/src
```

If you use the python/install.py script, you need to invoke it every time you rebuild LAMMPS (as a shared library) or make changes to the python/lammps.py file.

You can invoke install.py from the python directory as

```
% python install.py [libdir] [pydir]
```

The optional libdir is where to copy the LAMMPS shared library to; the default is /usr/local/lib. The optional pydir is where to copy the lammps.py file to; the default is the site-packages directory of the version of Python that is running the install script.
Note that libdir must be a location that is in your default LD_LIBRARY_PATH, like /usr/local/lib or /usr/lib. And pydir must be a location that Python looks in by default for imported modules, like its site-packages dir. If you want to copy these files to non-standard locations, such as within your own user space, you will need to set your PYTHONPATH and LD_LIBRARY_PATH environment variables accordingly, as above.

If the install.py script does not allow you to copy files into system directories, prefix the python command with "sudo". If you do this, make sure that the Python that root runs is the same as the Python you run. E.g. you may need to do something like

```bash
% sudo /usr/local/bin/python install.py [libdir] [pydir]
```

You can also invoke install.py from the make command in the src directory as

```bash
% make install-python
```

In this mode you cannot append optional arguments. Again, you may need to prefix this with "sudo". In this mode you cannot control which Python is invoked by root.

Note that if you want Python to be able to load different versions of the LAMMPS shared library (see this section below), you will need to manually copy files like lmplammps_g++.so into the appropriate system directory. This is not needed if you set the LD_LIBRARY_PATH environment variable as described above.

### 11.3 Extending Python with MPI to run in parallel

If you wish to run LAMMPS in parallel from Python, you need to extend your Python with an interface to MPI. This also allows you to make MPI calls directly from Python in your script, if you desire.

There are several Python packages available that purport to wrap MPI as a library and allow MPI functions to be called from Python.

These include

- pyMPI
- maroonmpi
- mpi4py
- myMPI
- Pypar

All of these except pyMPI work by wrapping the MPI library and exposing (some portion of) its interface to your Python script. This means Python cannot be used interactively in parallel, since they do not address the issue of interactive input to multiple instances of Python running on different processors. The one exception is pyMPI, which alters the Python interpreter to address this issue, and (I believe) creates a new alternate executable (in place of "python" itself) as a result.

In principle any of these Python/MPI packages should work to invoke LAMMPS in parallel and MPI calls themselves from a Python script which is itself running in parallel. However, when I downloaded and looked at a few of them, their documentation was incomplete and I had trouble with their installation. It's not clear if some of the packages are still being actively developed and supported.

The one I recommend, since I have successfully used it with LAMMPS, is Pypar. Pypar requires the ubiquitous Numpy package be installed in your Python. After launching python, type
import numpy

to see if it is installed. If not, here is how to install it (version 1.3.0b1 as of April 2009). Unpack the numpy tarball and from its top-level directory, type

```bash
python setup.py build
sudo python setup.py install
```

The "sudo" is only needed if required to copy Numpy files into your Python distribution's site-packages directory.

To install Pypar (version pypar-2.1.4_94 as of Aug 2012), unpack it and from its "source" directory, type

```bash
python setup.py build
sudo python setup.py install
```

Again, the "sudo" is only needed if required to copy Pypar files into your Python distribution's site-packages directory.

If you have successfully installed Pypar, you should be able to run Python and type

```python
import pypar
```

without error. You should also be able to run python in parallel on a simple test script

```bash
% mpirun -np 4 python test.py
```

where test.py contains the lines

```python
import pypar
print "Proc %d out of %d procs" % (pypar.rank(),pypar.size())
```

and see one line of output for each processor you run on.

IMPORTANT NOTE: To use Pypar and LAMMPS in parallel from Python, you must insure both are using the same version of MPI. If you only have one MPI installed on your system, this is not an issue, but it can be if you have multiple MPIS. Your LAMMPS build is explicit about which MPI it is using, since you specify the details in your lo-level src/MAKE/Makefile.foo file. Pypar uses the "mpicc" command to find information about the MPI it uses to build against. And it tries to load "libmpi.so" from the LD_LIBRARY_PATH. This may or may not find the MPI library that LAMMPS is using. If you have problems running both Pypar and LAMMPS together, this is an issue you may need to address, e.g. by moving other MPI installations so that Pypar finds the right one.

### 11.4 Testing the Python-LAMMPS interface

To test if LAMMPS is callable from Python, launch Python interactively and type:

```python
>>> from lammps import lammps
>>> lmp = lammps()
```

If you get no errors, you're ready to use LAMMPS from Python. If the 2nd command fails, the most common error to see is

```bash
OSError: Could not load LAMMPS dynamic library
```
which means Python was unable to load the LAMMPS shared library. This typically occurs if the system can't find the LAMMPS shared library or one of the auxiliary shared libraries it depends on, or if something about the library is incompatible with your Python. The error message should give you an indication of what went wrong.

You can also test the load directly in Python as follows, without first importing from the lammps.py file:

```python
>>> from ctypes import CDLL
>>> CDLL("liblammps.so")
```

If an error occurs, carefully go thru the steps in Section 5 and above about building a shared library and about insuring Python can find the necessary two files it needs.

**Test LAMMPS and Python in serial:**

To run a LAMMPS test in serial, type these lines into Python interactively from the bench directory:

```python
>>> from lammps import lammps
>>> lmp = lammps()  
>>> lmp.file("in.lj")
```

Or put the same lines in the file test.py and run it as

```
% python test.py
```

Either way, you should see the results of running the in.lj benchmark on a single processor appear on the screen, the same as if you had typed something like:

```
lmp_g++ <in.lj
```

**Test LAMMPS and Python in parallel:**

To run LAMMPS in parallel, assuming you have installed the Pypar package as discussed above, create a test.py file containing these lines:

```python
import pypar
from lammps import lammps
lmp = lammps()
lmp.file("in.lj")
print "Proc %d out of %d procs has" % (pypar.rank(),pypar.size()), lmp
pypar.finalize()
```

You can then run it in parallel as:

```
% mpirun -np 4 python test.py
```

and you should see the same output as if you had typed

```
% mpirun -np 4 lmp_g++ <in.lj
```

Note that if you leave out the 3 lines from test.py that specify Pypar commands you will instantiate and run LAMMPS independently on each of the P processors specified in the mpirun command. In this case you should get 4 sets of output, each showing that a LAMMPS run was made on a single processor, instead of one set of output showing that LAMMPS ran on 4 processors. If the 1-processor outputs occur, it means that Pypar is not working correctly.
Also note that once you import the PyPar module, Pypar initializes MPI for you, and you can use MPI calls directly in your Python script, as described in the Pypar documentation. The last line of your Python script should be pypar.finalize(), to insure MPI is shut down correctly.

Running Python scripts:

Note that any Python script (not just for LAMMPS) can be invoked in one of several ways:

% python foo.script
% python -i foo.script
% foo.script

The last command requires that the first line of the script be something like this:

#!/usr/local/bin/python
#!/usr/local/bin/python -i

where the path points to where you have Python installed, and that you have made the script file executable:

% chmod +x foo.script

Without the "-i" flag, Python will exit when the script finishes. With the "-i" flag, you will be left in the Python interpreter when the script finishes, so you can type subsequent commands. As mentioned above, you can only run Python interactively when running Python on a single processor, not in parallel.

11.5 Using LAMMPS from Python

The Python interface to LAMMPS consists of a Python "lammps" module, the source code for which is in python/lammps.py, which creates a "lammps" object, with a set of methods that can be invoked on that object. The sample Python code below assumes you have first imported the "lammps" module in your Python script, as follows:

from lammps import lammps

These are the methods defined by the lammps module. If you look at the file src/library.cpp you will see that they correspond one-to-one with calls you can make to the LAMMPS library from a C++ or C or Fortran program.

lmp = lammps()           # create a LAMMPS object using the default liblammps.so library
lmp = lammps("g++")      # create a LAMMPS object using the liblammps_g++.so library
lmp = lammps("",list)    # ditto, with command-line args, e.g. list = ["-echo","screen"]

lmp.close()              # destroy a LAMMPS object

lmp.file(file)           # run an entire input script, file = "in.lj"

lmp.command(cmd)         # invoke a single LAMMPS command, cmd = "run 100"

xlo = lmp.extract_global(name,type)  # extract a global quantity
# name = "boxxlo", "nlocal", etc
# type = 0 = int
# 1 = double

cords = lmp.extract_atom(name,type)    # extract a per-atom quantity
# name = "x", "type", etc
# type = 0 = vector of ints  
#        1 = array of ints  
#        2 = vector of doubles  
#        3 = array of doubles

ing = lmp.extract_compute(id,style,type)  # extract value(s) from a compute  
v3 = lmp.extract_fix(id,style,type,i,j)   # extract value(s) from a fix  
# id = ID of compute or fix  
# style = 0 = global data  
#         1 = per-atom data  
#         2 = local data  
# type = 0 = scalar  
#        1 = vector  
#        2 = array  
# i,j = indices of value in global vector or array

var = lmp.extract_variable(name,group,flag)  # extract value(s) from a variable  
# name = name of variable  
# group = group ID (ignored for equal-style variables)  
# flag = 0 = equal-style variable  
#        1 = atom-style variable

natoms = lmp.get_natoms()  # total # of atoms as int

data = lmp.gather_atoms(name,type,count)  # return atom attribute of all atoms gathered into data, ordered by atom ID  
# name = "x", "charge", "type", etc  
# count = # of per-atom values, 1 or 3, etc

lmp.scatter_atoms(name,type,count,data)  # scatter atom attribute of all atoms from data, ordered by atom ID  
# name = "x", "charge", "type", etc  
# count = # of per-atom values, 1 or 3, etc

IMPORTANT NOTE: Currently, the creation of a LAMMPS object from within lammps.py does not take an MPI communicator as an argument. There should be a way to do this, so that the LAMMPS instance runs on a subset of processors if desired, but I don’t know how to do it from Pypar. So for now, it runs with MPI_COMM_WORLD, which is all the processors. If someone figures out how to do this with one or more of the Python wrappers for MPI, like Pypar, please let us know and we will amend these doc pages.

Note that you can create multiple LAMMPS objects in your Python script, and coordinate and run multiple simulations, e.g.

```python
from lammps import lammps
lmp1 = lammps()
lmp2 = lammps()
lmp1.file("in.file1")
lmp2.file("in.file2")
```

The file() and command() methods allow an input script or single commands to be invoked.

The extract_global(), extract_atom(), extract_compute(), extract_fix(), and extract_variable() methods return values or pointers to data structures internal to LAMMPS.

For extract_global() see the src/library.cpp file for the list of valid names. New names could easily be added. A double or integer is returned. You need to specify the appropriate data type via the type argument.

For extract_atom(), a pointer to internal LAMMPS atom-based data is returned, which you can use via normal Python subscripting. See the extract() method in the src/atom.cpp file for a list of valid names. Again, new names could easily be added. A pointer to a vector of doubles or integers, or a pointer to an array of doubles (double **) or integers (int **) is returned. You need to specify the appropriate data type via the type argument.
For extract_compute() and extract_fix(), the global, per-atom, or local data calculated by the compute or fix can be accessed. What is returned depends on whether the compute or fix calculates a scalar or vector or array. For a scalar, a single double value is returned. If the compute or fix calculates a vector or array, a pointer to the internal LAMMPS data is returned, which you can use via normal Python subscripting. The one exception is that for a fix that calculates a global vector or array, a single double value from the vector or array is returned, indexed by I (vector) or I and J (array). I,J are zero-based indices. The I,J arguments can be left out if not needed. See Section_howto 15 of the manual for a discussion of global, per-atom, and local data, and of scalar, vector, and array data types. See the doc pages for individual computes and fixes for a description of what they calculate and store.

For extract_variable(), an equal-style or atom-style variable is evaluated and its result returned.

For equal-style variables a single double value is returned and the group argument is ignored. For atom-style variables, a vector of doubles is returned, one value per atom, which you can use via normal Python subscripting. The values will be zero for atoms not in the specified group.

The get_natoms() method returns the total number of atoms in the simulation, as an int.

The gather_atoms() method returns a ctypes vector of ints or doubles as specified by type, of length count*natoms, for the property of all the atoms in the simulation specified by name, ordered by count and then by atom ID. The vector can be used via normal Python subscripting. If atom IDs are not consecutively ordered within LAMMPS, a None is returned as indication of an error.

Note that the data structure gather_atoms("x") returns is different from the data structure returned by extract_atom("x") in four ways. (1) Gather_atoms() returns a vector which you index as x[i]; extract_atom() returns an array which you index as x[i][j]. (2) Gather_atoms() orders the atoms by atom ID while extract_atom() does not. (3) Gather_atoms() returns a list of all atoms in the simulation; extract_atom() returns just the atoms local to each processor. (4) Finally, the gather_atoms() data structure is a copy of the atom coords stored internally in LAMMPS, whereas extract_atom() returns an array that effectively points directly to the internal data. This means you can change values inside LAMMPS from Python by assigning a new values to the gather_atoms() array. To do this with the gather_atoms() vector, you need to change values in the vector, then invoke the scatter_atoms() method.

The scatter_atoms() method takes a vector of ints or doubles as specified by type, of length count*natoms, for the property of all the atoms in the simulation specified by name, ordered by count and then by atom ID. It uses the vector of data to overwrite the corresponding properties for each atom inside LAMMPS. This requires LAMMPS to have its "map" option enabled; see the atom_modify command for details. If it is not, or if atom IDs are not consecutively ordered, no coordinates are reset.

The array of coordinates passed to scatter_atoms() must be a ctypes vector of ints or doubles, allocated and initialized something like this:

```python
from ctypes import *

natoms = lmp.get_natoms()
n3 = 3*natoms
x = (n3*c_double)()
x0 = x coord of atom with ID 1
x1 = y coord of atom with ID 1
x2 = z coord of atom with ID 1
x3 = x coord of atom with ID 2
...
xn3-1 = z coord of atom with ID natoms
lmp.scatter_coords("x",1,3,x)
```
Alternatively, you can just change values in the vector returned by `gather_atoms("x",1,3)`, since it is a ctypes vector of doubles.

As noted above, these Python class methods correspond one-to-one with the functions in the LAMMPS library interface in src/library.cpp and library.h. This means you can extend the Python wrapper via the following steps:

- Add a new interface function to src/library.cpp and src/library.h.
- Rebuild LAMMPS as a shared library.
- Add a wrapper method to python/lammps.py for this interface function.
- You should now be able to invoke the new interface function from a Python script. Isn’t ctypes amazing?

### 11.6 Example Python scripts that use LAMMPS

These are the Python scripts included as demos in the python/examples directory of the LAMMPS distribution, to illustrate the kinds of things that are possible when Python wraps LAMMPS. If you create your own scripts, send them to us and we can include them in the LAMMPS distribution.

<table>
<thead>
<tr>
<th>Script</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>trivial.py</td>
<td>read/run a LAMMPS input script thru Python</td>
</tr>
<tr>
<td>demo.py</td>
<td>invoke various LAMMPS library interface routines</td>
</tr>
<tr>
<td>simple.py</td>
<td>mimic operation of couple/simple/simple.cpp in Python</td>
</tr>
<tr>
<td>gui.py</td>
<td>GUI go/stop/temperature-slider to control LAMMPS</td>
</tr>
<tr>
<td>plot.py</td>
<td>real-time temperature plot with GnuPlot via Pizza.py</td>
</tr>
<tr>
<td>viz_tool.py</td>
<td>real-time viz via some viz package</td>
</tr>
<tr>
<td>vizplotgui_tool.py</td>
<td>combination of viz_tool.py and plot.py and gui.py</td>
</tr>
</tbody>
</table>

For the `viz_tool.py` and `vizplotgui_tool.py` commands, replace "tool" with "gl" or "atomeye" or "pymol" or "vmd", depending on what visualization package you have installed.

Note that for GL, you need to be able to run the Pizza.py GL tool, which is included in the pizza sub-directory. See the Pizza.py doc pages for more info:

Note that for AtomEye, you need version 3, and there is a line in the scripts that specifies the path and name of the executable. See the AtomEye WWW pages [here](http://mt.seas.upenn.edu/Archive/Graphics/A3/A3.html) or [here](http://mt.seas.upenn.edu/Archive/Graphics/A) for more details:

Note that for PyMol, you need to have built and installed the open-source version of PyMol in your Python, so that you can import it from a Python script. See the PyMol WWW pages [here](http://www.pymol.org) or [here](http://sourceforge.net/scm/?type=svn&group_id=4546) for more details:

The latter link is to the open-source version.

Note that for VMD, you need a fairly current version (1.8.7 works for me) and there are some lines in the `pizza/vmd.py` script for 4 PIZZA variables that have to match the VMD installation on your system.
See the python/README file for instructions on how to run them and the source code for individual scripts for comments about what they do.

Here are screenshots of the vizplotgui_tool.py script in action for different visualization package options. Click to see larger images:
12. Errors

This section describes the errors you can encounter when using LAMMPS, either conceptually, or as printed out by the program.

12.1 Common problems
12.2 Reporting bugs
12.3 Error & warning messages

12.1 Common problems

If two LAMMPS runs do not produce the same answer on different machines or different numbers of processors, this is typically not a bug. In theory you should get identical answers on any number of processors and on any machine. In practice, numerical round-off can cause slight differences and eventual divergence of molecular dynamics phase space trajectories within a few 100s or few 1000s of timesteps. However, the statistical properties of the two runs (e.g. average energy or temperature) should still be the same.

If the velocity command is used to set initial atom velocities, a particular atom can be assigned a different velocity when the problem is run on a different number of processors or on different machines. If this happens, the phase space trajectories of the two simulations will rapidly diverge. See the discussion of the loop option in the velocity command for details and options that avoid this issue.

Similarly, the create_atoms command generates a lattice of atoms. For the same physical system, the ordering and numbering of atoms by atom ID may be different depending on the number of processors.

Some commands use random number generators which may be setup to produce different random number streams on each processor and hence will produce different effects when run on different numbers of processors. A commonly-used example is the fix langevin command for thermostatting.

A LAMMPS simulation typically has two stages, setup and run. Most LAMMPS errors are detected at setup time; others like a bond stretching too far may not occur until the middle of a run.

LAMMPS tries to flag errors and print informative error messages so you can fix the problem. Of course, LAMMPS cannot figure out your physics or numerical mistakes, like choosing too big a timestep, specifying erroneous force field coefficients, or putting 2 atoms on top of each other! If you run into errors that LAMMPS doesn't catch that you think it should flag, please send an email to the developers.

If you get an error message about an invalid command in your input script, you can determine what command is causing the problem by looking in the log.lammps file or using the echo command to see it on the screen. For a given command, LAMMPS expects certain arguments in a specified order. If you mess this up, LAMMPS will often flag the error, but it may read a bogus argument and assign a value that is valid, but not what you wanted. E.g. trying to read the string "abc" as an integer value and assigning the associated variable a value of 0.

If you get an error message about an invalid command in your input script, you can determine what command is causing the problem by looking in the log.lammps file or using the echo command to see it on the screen. For a given command, LAMMPS expects certain arguments in a specified order. If you mess this up, LAMMPS will often flag the error, but it may read a bogus argument and assign a value that is valid, but not what you wanted. E.g. trying to read the string "abc" as an integer value and assigning the associated variable a value of 0.

Generally, LAMMPS will print a message to the screen and logfile and exit gracefully when it encounters a fatal error. Sometimes it will print a WARNING to the screen and logfile and continue on; you can decide if the WARNING is important or not. A WARNING message that is generated in the middle of a run is only printed to the screen, not to the logfile, to avoid cluttering up thermodynamic output. If LAMMPS crashes or hangs without spitting out an error message first then it could be a bug (see this section) or one of the following cases:
LAMMPS runs in the available memory a processor allows to be allocated. Most reasonable MD runs are compute limited, not memory limited, so this shouldn't be a bottleneck on most platforms. Almost all large memory allocations in the code are done via C-style malloc's which will generate an error message if you run out of memory. Smaller chunks of memory are allocated via C++ "new" statements. If you are unlucky you could run out of memory just when one of these small requests is made, in which case the code will crash or hang (in parallel), since LAMMPS doesn't trap on those errors.

Illegal arithmetic can cause LAMMPS to run slow or crash. This is typically due to invalid physics and numerics that your simulation is computing. If you see wild thermodynamic values or NaN values in your LAMMPS output, something is wrong with your simulation. If you suspect this is happening, it is a good idea to print out thermodynamic info frequently (e.g. every timestep) via the thermo so you can monitor what is happening. Visualizing the atom movement is also a good idea to insure your model is behaving as you expect.

In parallel, one way LAMMPS can hang is due to how different MPI implementations handle buffering of messages. If the code hangs without an error message, it may be that you need to specify an MPI setting or two (usually via an environment variable) to enable buffering or boost the sizes of messages that can be buffered.

### 12.2 Reporting bugs

If you are confident that you have found a bug in LAMMPS, follow these steps.

Check the New features and bug fixes section of the LAMMPS WWW site to see if the bug has already been reported or fixed or the Unfixed bug to see if a fix is pending.

Check the mailing list to see if it has been discussed before.

If not, send an email to the mailing list describing the problem with any ideas you have as to what is causing it or where in the code the problem might be. The developers will ask for more info if needed, such as an input script or data files.

The most useful thing you can do to help us fix the bug is to isolate the problem. Run it on the smallest number of atoms and fewest number of processors and with the simplest input script that reproduces the bug and try to identify what command or combination of commands is causing the problem.

As a last resort, you can send an email directly to the developers.

### 12.3 Error & warning messages

These are two alphabetic lists of the ERROR and WARNING messages LAMMPS prints out and the reason why. If the explanation here is not sufficient, the documentation for the offending command may help. Error and warning messages also list the source file and line number where the error was generated. For example, this message

ERROR: Illegal velocity command (velocity.cpp:78)

means that line #78 in the file src/velocity.cpp generated the error. Looking in the source code may help you figure out what went wrong.

Note that error messages from user-contributed packages are not listed here. If such an error occurs and is not self-explanatory, you'll need to look in the source code or contact the author of the package.
Errors:

1-3 bond count is inconsistent
An inconsistency was detected when computing the number of 1-3 neighbors for each atom. This likely means something is wrong with the bond topologies you have defined.

1-4 bond count is inconsistent
An inconsistency was detected when computing the number of 1-4 neighbors for each atom. This likely means something is wrong with the bond topologies you have defined.

64-bit atom IDs are not yet supported
See description of this data type in src/lmptype.h.

Accelerator sharing is not currently supported on system
Multiple MPI processes cannot share the accelerator on your system. For NVIDIA GPUs, see the nvidia-smi command to change this setting.

All angle coeffs are not set
All angle coefficients must be set in the data file or by the angle_coeff command before running a simulation.

All bond coeffs are not set
All bond coefficients must be set in the data file or by the bond_coeff command before running a simulation.

All dihedral coeffs are not set
All dihedral coefficients must be set in the data file or by the dihedral_coeff command before running a simulation.

All improper coeffs are not set
All improper coefficients must be set in the data file or by the improper_coeff command before running a simulation.

All masses are not set
For atom styles that define masses for each atom type, all masses must be set in the data file or by the mass command before running a simulation. They must also be set before using the velocity command.

All pair coeffs are not set
All pair coefficients must be set in the data file or by the pair_coeff command before running a simulation.

All read_dump x,y,z fields must be specified for scaled, triclinic coords
For triclinic boxes and scaled coordinates you must specify all 3 of the x,y,z fields, else LAMMPS cannot reconstruct the unscaled coordinates.

All universe/uloop variables must have same # of values
Self-explanatory.

All variables in next command must be same style
Self-explanatory.

Angle atom missing in delete_bonds
The delete_bonds command cannot find one or more atoms in a particular angle on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid angle.

Angle atom missing in set command
The set command cannot find one or more atoms in a particular angle on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid angle.

Angle atoms %d %d %d missing on proc %d at step %ld
One or more of 3 atoms needed to compute a particular angle are missing on this processor. Typically this is because the pairwise cutoff is set too short or the angle has blown apart and an atom is too far away.

Angle coeff for hybrid has invalid style
Angle style hybrid uses another angle style as one of its coefficients. The angle style used in the angle_coeff command or read from a restart file is not recognized.

Angle coeffs are not set
No angle coefficients have been assigned in the data file or via the angle_coeff command.
Angle potential must be defined for SHAKE
When shaking angles, an angle_style potential must be used.

Angle style hybrid cannot have hybrid as an argument
Self-explanatory.

Angle style hybrid cannot have none as an argument
Self-explanatory.

Angle style hybrid cannot use same pair style twice
Self-explanatory.

Angle table must range from 0 to 180 degrees
Self-explanatory.

Angle table parameters did not set N
List of angle table parameters must include N setting.

Angle_coeff command before angle_style is defined
Coefficients cannot be set in the data file or via the angle_coeff command until an angle_style has been assigned.

Angle_coeff command before simulation box is defined
The angle_coeff command cannot be used before a read_data, read_restart, or create_box command.

Angle_coeff command when no angles allowed
The chosen atom style does not allow for angles to be defined.

Angle_style command when no angles allowed
The chosen atom style does not allow for angles to be defined.

Angles assigned incorrectly
Angles read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Angles defined but no angle types
The data file header lists angles but no angle types.

Another input script is already being processed
Cannot attempt to open a 2nd input script, when the original file is still being processed.

Append boundary must be shrink/minimum
The boundary style of the face where atoms are added must be of type m (shrink/minimum).

Arccos of invalid value in variable formula
Argument of arccos() must be between -1 and 1.

Arcsin of invalid value in variable formula
Argument of arcsin() must be between -1 and 1.

Assigning ellipsoid parameters to non-ellipsoid atom
Self-explanatory.

Assigning line parameters to non-line atom
Self-explanatory.

Assigning tri parameters to non-tri atom
Self-explanatory.

Atom IDs must be consecutive for velocity create loop all
Self-explanatory.

Atom count changed in fix neb
This is not allowed in a NEB calculation.

Atom count is inconsistent, cannot write restart file
Sum of atoms across processors does not equal initial total count. This is probably because you have lost some atoms.

Atom in too many rigid bodies - boost MAXBODY
Fix poems has a parameter MAXBODY (in fix_poems.cpp) which determines the maximum number of rigid bodies a single atom can belong to (i.e. a multibody joint). The bodies you have defined exceed this limit.

Atom sort did not operate correctly
This is an internal LAMMPS error. Please report it to the developers.

Atom sorting has bin size = 0.0
   The neighbor cutoff is being used as the bin size, but it is zero. Thus you must explicitly list a bin size in
   the atom_modify sort command or turn off sorting.

Atom style hybrid cannot have hybrid as an argument
   Self-explanatory.

Atom style hybrid cannot use same atom style twice
   Self-explanatory.

Atom vector in equal-style variable formula
   Atom vectors generate one value per atom which is not allowed in an equal-style variable.

Atom-style variable in equal-style variable formula
   Atom-style variables generate one value per atom which is not allowed in an equal-style variable.

Atom_modify map command after simulation box is defined
   The atom_modify map command cannot be used after a read_data, read_restart, or create_box command.

Atom_modify sort and first options cannot be used together
   Self-explanatory.

Atom_style command after simulation box is defined
   The atom_style command cannot be used after a read_data, read_restart, or create_box command.

Atom_style line can only be used in 2d simulations
   Self-explanatory.

Atom_style tri can only be used in 3d simulations
   Self-explanatory.

Attempt to pop empty stack in fix box/relax
   Internal LAMMPS error. Please report it to the developers.

Attempt to push beyond stack limit in fix box/relax
   Internal LAMMPS error. Please report it to the developers.

Attempting to rescale a 0.0 temperature
   Cannot rescale a temperature that is already 0.0.

Bad FENE bond
   Two atoms in a FENE bond have become so far apart that the bond cannot be computed.

Bad TIP4P angle type for PPPM/TIP4P
   Specified angle type is not valid.

Bad TIP4P bond type for PPPM/TIP4P
   Specified bond type is not valid.

Bad fix ID in fix append/atoms command
   The value of the fix_id for keyword spatial must start with the suffix f_.

Bad grid of processors
   The 3d grid of processors defined by the processors command does not match the number of processors
   LAMMPS is being run on.

Bad kspace_modify slab parameter
   KSpace_modify value for the slab/volume keyword must be >= 2.0.

Bad matrix inversion in mldivide3
   This error should not occur unless the matrix is badly formed.

Bad principal moments
   Fix rigid did not compute the principal moments of inertia of a rigid group of atoms correctly.

Bad quadratic solve for particle/line collision
   This is an internal error. It should normally not occur.

Bad quadratic solve for particle/tri collision
   This is an internal error. It should normally not occur.

Balance command before simulation box is defined
   The balance command cannot be used before a read_data, read_restart, or create_box command.

Balance dynamic string is invalid
The string can only contain the characters "x", "y", or "z".

**Balance produced bad splits**
This should not occur. It means two or more cutting plane locations are on top of each other or out of order. Report the problem to the developers.

**Bias compute does not calculate a velocity bias**
The specified compute must compute a bias for temperature.

**Bias compute does not calculate temperature**
The specified compute must compute temperature.

**Bias compute group does not match compute group**
The specified compute must operate on the same group as the parent compute.

**Big particle in fix srd cannot be point particle**
Big particles must be extended spheriods or ellipsoids.

**Bigint setting in lmptype.h is invalid**
Size of bigint is less than size of tagint.

**Bigint setting in lmptype.h is not compatible**
Bigint stored in restart file is not consistent with LAMMPS version you are running.

**Bitmapped lookup tables require int/float be same size**
Cannot use pair tables on this machine, because of word sizes. Use the pair_modify command with table 0 instead.

**Bitmapped table in file does not match requested table**
Setting for bitmapped table in pair_coeff command must match table in file exactly.

**Bitmapped table is incorrect length in table file**
Number of table entries is not a correct power of 2.

**Bond and angle potentials must be defined for TIP4P**
Cannot use TIP4P pair potential unless bond and angle potentials are defined.

**Bond atom missing in box size check**
The 2nd atoms needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

**Bond atom missing in delete_bonds**
The delete_bonds command cannot find one or more atoms in a particular bond on a particular processor.
The pairwise cutoff is too short or the atoms are too far apart to make a valid bond.

**Bond atom missing in set command**
The set command cannot find one or more atoms in a particular bond on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid bond.

**Bond atoms %d %d missing on proc %d at step %ld**
One or both of 2 atoms needed to compute a particular bond are missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

**Bond coeff for hybrid has invalid style**
Bond style hybrid uses another bond style as one of its coefficients. The bond style used in the bond_coeff command or read from a restart file is not recognized.

**Bond coeffs are not set**
No bond coefficients have been assigned in the data file or via the bond_coeff command.

**Bond potential must be defined for SHAKE**
Cannot use fix shake unless bond potential is defined.

**Bond style hybrid cannot have hybrid as an argument**
Self-explanatory.

**Bond style hybrid cannot have none as an argument**
Self-explanatory.

**Bond style hybrid cannot use same pair style twice**
Self-explanatory.

**Bond style quartic cannot be used with 3,4-body interactions**
No angle, dihedral, or improper styles can be defined when using bond style quartic.
Bond style quartic requires special_bonds = 1,1,1
This is a restriction of the current bond quartic implementation.

Bond table parameters did not set N
List of bond table parameters must include N setting.

Bond table values are not increasing
The values in the tabulated file must be monotonically increasing.

Bond/angle/dihedral extent > half of periodic box length
This is a restriction because LAMMPS can be confused about which image of an atom in the bonded interaction is the correct one to use. "Extent" in this context means the maximum end-to-end length of the bond/angle/dihedral. LAMMPS computes this by taking the maximum bond length, multiplying by the number of bonds in the interaction (e.g. 3 for a dihedral) and adding a small amount of stretch.

Bond_coeff command before bond_style is defined
Coefficients cannot be set in the data file or via the bond_coeff command until an bond_style has been assigned.

Bond_coeff command before simulation box is defined
The bond_coeff command cannot be used before a read_data, read_restart, or create_box command.

Bond_coeff command when no bonds allowed
The chosen atom style does not allow for bonds to be defined.

Bond_style command when no bonds allowed
The chosen atom style does not allow for bonds to be defined.

Bonds assigned incorrectly
Bonds read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Bonds defined but no bond types
The data file header lists bonds but no bond types.

Both sides of boundary must be periodic
Cannot specify a boundary as periodic only on the lo or hi side. Must be periodic on both sides.

Boundary command after simulation box is defined
The boundary command cannot be used after a read_data, read_restart, or create_box command.

Box bounds are invalid
The box boundaries specified in the read_data file are invalid. The lo value must be less than the hi value for all 3 dimensions.

Can not specify Pxy/Pxz/Pyz in fix box/relax with non-triclinic box
Only triclinic boxes can be used with off-diagonal pressure components. See the region prism command for details.

Can not specify Pxy/Pxz/Pyz in fix nvt/npt/nph with non-triclinic box
Only triclinic boxes can be used with off-diagonal pressure components. See the region prism command for details.

Can only use -plog with multiple partitions
Self-explanatory. See doc page discussion of command-line switches.

Can only use -pscreen with multiple partitions
Self-explanatory. See doc page discussion of command-line switches.

Can only use NEB with 1-processor replicas
This is current restriction for NEB as implemented in LAMMPS.

Can only use TAD with 1-processor replicas for NEB
This is current restriction for NEB as implemented in LAMMPS.

Cannot (yet) use K-space slab correction with compute group/group
This option is not yet supported.

Cannot (yet) use Kspace slab correction with compute group/group
This option is not yet supported.

Cannot (yet) use PPPM with triclinic box
This feature is not yet supported.
Cannot add atoms to fix move variable
Atoms can not be added afterwards to this fix option.

Cannot append atoms to a triclinic box
The simulation box must be defined with edges aligned with the Cartesian axes.

Cannot balance in z dimension for 2d simulation
Self-explanatory.

Cannot change box ortho/triclinic with certain fixes defined
This is because those fixes store the shape of the box. You need to use unfix to discard the fix, change the box, then redefine a new fix.

Cannot change box ortho/triclinic with dumps defined
This is because some dumps store the shape of the box. You need to use undump to discard the dump, change the box, then redefine a new dump.

Cannot change box tilt factors for orthogonal box
Cannot use tilt factors unless the simulation box is non-orthogonal.

Cannot change box to orthogonal when tilt is non-zero
Self-explanatory.

Cannot change box z boundary to nonperiodic for a 2d simulation
Self-explanatory.

Cannot change dump_modify every for dump dcd
The frequency of writing dump dcd snapshots cannot be changed.

Cannot change dump_modify every for dump xtc
The frequency of writing dump xtc snapshots cannot be changed.

Cannot change timestep once fix srd is setup
This is because various SRD properties depend on the timestep size.

Cannot change timestep with fix pour
This fix pre-computes some values based on the timestep, so it cannot be changed during a simulation run.

Cannot change box after reading restart file with per-atom info
This is because the restart file info cannot be migrated with the atoms. You can get around this by performing a 0-timestep run which will assign the restart file info to actual atoms.

Cannot change box in xz or yz for 2d simulation
Self-explanatory.

Cannot change box in z dimension for 2d simulation
Self-explanatory.

Cannot compute PPPM G
LAMMPS failed to compute a valid approximation for the PPPM g_ewald factor that partitions the computation between real space and k-space.

Cannot create an atom map unless atoms have IDs
The simulation requires a mapping from global atom IDs to local atoms, but the atoms that have been defined have no IDs.

Cannot create atoms with undefined lattice
Must use the lattice command before using the create_atoms command.

Cannot create/grow a vector/array of pointers for %s
LAMMPS code is making an illegal call to the templated memory allocaters, to create a vector or array of pointers.

Cannot create_atoms after reading restart file with per-atom info
The per-atom info was stored to be used when by a fix that you may re-define. If you add atoms before re-defining the fix, then there will not be a correct amount of per-atom info.

Cannot create_box after simulation box is defined
The create_box command cannot be used after a read_data, read_restart, or create_box command.

Cannot currently use pair reax with pair hybrid
This is not yet supported.
Cannot delete group all
Self-explanatory.

Cannot delete group currently used by a compute
Self-explanatory.

Cannot delete group currently used by a dump
Self-explanatory.

Cannot delete group currently used by a fix
Self-explanatory.

Cannot delete group currently used by atom_modify first
Self-explanatory.

Cannot displace_atoms after reading restart file with per-atom info
This is because the restart file info cannot be migrated with the atoms. You can get around this by
performing a 0-timestep run which will assign the restart file info to actual atoms.

Cannot do GCMC on atoms in atom_modify first group
This is a restriction due to the way atoms are organized in a list to enable the atom_modify first
command.

Cannot dump JPG file
LAMMPS was not built with the -DLAMMPS_JPEG switch in the Makefile.

Cannot dump sort on atom IDs with no atom IDs defined
Self-explanatory.

Cannot evaporate atoms in atom_modify first group
This is a restriction due to the way atoms are organized in a list to enable the atom_modify first
command.

Cannot find delete_bonds group ID
Group ID used in the delete_bonds command does not exist.

Cannot have both pair_modify shift and tail set to yes
These 2 options are contradictory.

Cannot open -reorder file
Self-explanatory.

Cannot open ADP potential file %s
The specified ADP potential file cannot be opened. Check that the path and name are correct.

Cannot open AIREBO potential file %s
The specified AIREBO potential file cannot be opened. Check that the path and name are correct.

Cannot open BOP potential file %s
The specified BOP potential file cannot be opened. Check that the path and name are correct.

Cannot open COMB potential file %s
The specified COMB potential file cannot be opened. Check that the path and name are correct.

Cannot open EAM potential file %s
The specified EAM potential file cannot be opened. Check that the path and name are correct.

Cannot open EIM potential file %s
The specified EIM potential file cannot be opened. Check that the path and name are correct.

Cannot open LCBOP potential file %s
The specified LCBOP potential file cannot be opened. Check that the path and name are correct.

Cannot open MEAM potential file %s
The specified MEAM potential file cannot be opened. Check that the path and name are correct.

Cannot open Stillinger-Weber potential file %s
The specified SW potential file cannot be opened. Check that the path and name are correct.

Cannot open Tersoff potential file %s
The specified Tersoff potential file cannot be opened. Check that the path and name are correct.

Cannot open balance output file
Self-explanatory.

Cannot open custom file

Self-explanatory.

**Cannot open dir to search for restart file**

Using a "*" in the name of the restart file will open the current directory to search for matching file names.

**Cannot open dump file**

The output file for the dump command cannot be opened. Check that the path and name are correct.

**Cannot open file %s**

The specified file cannot be opened. Check that the path and name are correct.

**Cannot open fix ave/correlate file %s**

The specified file cannot be opened. Check that the path and name are correct.

**Cannot open fix ave/histo file %s**

The specified file cannot be opened. Check that the path and name are correct.

**Cannot open fix ave/spatial file %s**

The specified file cannot be opened. Check that the path and name are correct.

**Cannot open fix ave/time file %s**

The specified file cannot be opened. Check that the path and name are correct.

**Cannot open fix balance output file**

Self-explanatory.

**Cannot open fix poems file %s**

The specified file cannot be opened. Check that the path and name are correct.

**Cannot open fix print file %s**

The output file generated by the fix print command cannot be opened.

**Cannot open fix qeq/comb file %s**

The output file for the fix qeq/combs command cannot be opened. Check that the path and name are correct.

**Cannot open fix reax/bonds file %s**

The output file for the fix reax/bonds command cannot be opened. Check that the path and name are correct.

**Cannot open fix rigid infile %s**

The specified file cannot be opened. Check that the path and name are correct.

**Cannot open fix tmd file %s**

The output file for the fix tmd command cannot be opened. Check that the path and name are correct.

**Cannot open fix ttm file %s**

The output file for the fix ttm command cannot be opened. Check that the path and name are correct.

**Cannot open gzipped file**

LAMMPS is attempting to open a gzipped version of the specified file but was unsuccessful. Check that the path and name are correct.

**Cannot open input script %s**

Self-explanatory.

**Cannot open log.lammps**

The default LAMMPS log file cannot be opened. Check that the directory you are running in allows for files to be created.

**Cannot open logfile**

The LAMMPS log file named in a command-line argument cannot be opened. Check that the path and name are correct.

**Cannot open logfile %s**

The LAMMPS log file specified in the input script cannot be opened. Check that the path and name are correct.

**Cannot open pair_write file**

The specified output file for pair energies and forces cannot be opened. Check that the path and name are correct.

**Cannot open processors output file**
Cannot open restart file %s
Self-explanatory.

Cannot open screen file
The screen file specified as a command-line argument cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot open universe log file
For a multi-partition run, the master log file cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot open universe screen file
For a multi-partition run, the master screen file cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot read_data after simulation box is defined
The read_data command cannot be used after a read_data, read_restart, or create_box command.

Cannot read_restart after simulation box is defined
The read_restart command cannot be used after a read_data, read_restart, or create_box command.

Cannot redefine variable as a different style
An equal-style variable can be re-defined but only if it was originally an equal-style variable.

Cannot replicate 2d simulation in z dimension
The replicate command cannot replicate a 2d simulation in the z dimension.

Cannot replicate with fixes that store atom quantities
Either fixes are defined that create and store atom-based vectors or a restart file was read which included atom-based vectors for fixes. The replicate command cannot duplicate that information for new atoms.
You should use the replicate command before fixes are applied to the system.

Cannot reset timestep with a dynamic region defined
Dynamic regions (see the region command) have a time dependence. Thus you cannot change the timestep when one or more of these are defined.

Cannot reset timestep with a time-dependent fix defined
You cannot reset the timestep when a fix that keeps track of elapsed time is in place.

Cannot restart fix rigid/nvt with different # of chains
This is because the restart file contains per-chain info.

Cannot run 2d simulation with nonperiodic Z dimension
Use the boundary command to make the z dimension periodic in order to run a 2d simulation.

Cannot set both respa pair and inner/middle/outer
In the rRESPA integrator, you must compute pairwise potentials either all together (pair), or in pieces (inner/middle/outer). You can't do both.

Cannot set dump_modify flush for dump xtc
Self-explanatory.

Cannot set mass for this atom style
This atom style does not support mass settings for each atom type. Instead they are defined on a per-atom basis in the data file.

Cannot set meso_rho for this atom style
Self-explanatory.

Cannot set non-zero image flag for non-periodic dimension
Self-explanatory.

Cannot set non-zero z velocity for 2d simulation
Self-explanatory.

Cannot set quaternion for atom that has none
Self-explanatory.

Cannot set respa middle without inner/outer
In the rRESPA integrator, you must define both a inner and outer setting in order to use a middle setting.

Cannot set theta for atom that is not a line
Self-explanatory.

Cannot set this attribute for this atom style
The attribute being set does not exist for the defined atom style.

Cannot set variable z velocity for 2d simulation
Self-explanatory.

Cannot skew triclinic box in z for 2d simulation
Self-explanatory.

Cannot use -cuda on without USER-CUDA installed
The USER-CUDA package must be installed via "make yes-user-cuda" before LAMMPS is built.

Cannot use -reorder after -partition
Self-explanatory. See doc page discussion of command-line switches.

Cannot use Ewald with 2d simulation
The kspace style ewald cannot be used in 2d simulations. You can use 2d Ewald in a 3d simulation; see the kspace_modify command.

Cannot use Ewald with triclinic box
This feature is not yet supported.

Cannot use NEB unless atom map exists
Use the atom_modify command to create an atom map.

Cannot use NEB with a single replica
Self-explanatory.

Cannot use NEB with atom_modify sort enabled
This is a current restriction for NEB implemented in LAMMPS.

Cannot use PPPM with 2d simulation
The kspace style ppm cannot be used in 2d simulations. You can use 2d PPPM in a 3d simulation; see the kspace_modify command.

Cannot use PRD with a time-dependent fix defined
PRD alters the timestep in ways that will mess up these fixes.

Cannot use PRD with a time-dependent region defined
PRD alters the timestep in ways that will mess up these regions.

Cannot use PRD with atom_modify sort enabled
This is a current restriction of PRD. You must turn off sorting, which is enabled by default, via the atom_modify command.

Cannot use PRD with multi-processor replicas unless atom map exists
Use the atom_modify command to create an atom map.

Cannot use TAD unless atom map exists for NEB
See atom_modify map command to set this.

Cannot use TAD with a single replica for NEB
NEB requires multiple replicas.

Cannot use TAD with atom_modify sort enabled for NEB
This is a current restriction of NEB.

Cannot use a damped dynamics min style with fix box/relax
This is a current restriction in LAMMPS. Use another minimizer style.

Cannot use a damped dynamics min style with per-atom DOF
This is a current restriction in LAMMPS. Use another minimizer style.

Cannot use append/atoms in periodic dimension
The boundary style of the face where atoms are added can not be of type p (periodic).

Cannot use compute cluster/atom unless atoms have IDs
Atom IDs are used to identify clusters.

Cannot use cwiggle in variable formula between runs
This is a function of elapsed time.

Cannot use delete_atoms unless atoms have IDs
Your atoms do not have IDs, so the delete_atoms command cannot be used.
Cannot use delete_bonds with non-molecular system
   Your choice of atom style does not have bonds.

Cannot use fix GPU with USER-CUDA mode enabled
   You cannot use both the GPU and USER-CUDA packages together. Use one or the other.

Cannot use fix TMD unless atom map exists
   Using this fix requires the ability to lookup an atom index, which is provided by an atom map. An atom map does not exist (by default) for non-molecular problems. Using the atom_modify map command will force an atom map to be created.

Cannot use fix ave/spatial z for 2 dimensional model
   Self-explanatory.

Cannot use fix bond/break with non-molecular systems
   Self-explanatory.

Cannot use fix bond/create with non-molecular systems
   Self-explanatory.

Cannot use fix box/relax on a 2nd non-periodic dimension
   When specifying an off-diagonal pressure component, the 2nd of the two dimensions must be periodic.
   E.g. if the xy component is specified, then the y dimension must be periodic.

Cannot use fix box/relax on a non-periodic dimension
   When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix deform on a shrink-wrapped boundary
   The x, y, z options cannot be applied to shrink-wrapped dimensions.

Cannot use fix deform tilt on a shrink-wrapped 2nd dim
   This is because the shrink-wrapping will change the value of the strain implied by the tilt factor.

Cannot use fix deform trate on a box with zero tilt
   The trate style alters the current strain.

Cannot use fix enforce2d with 3d simulation
   Self-explanatory.

Cannot use fix msst without per-type mass defined
   Self-explanatory.

Cannot use fix npt and fix deform on same component of stress tensor
   This would be changing the same box dimension twice.

Cannot use fix nvt/npt/nph on a 2nd non-periodic dimension
   When specifying an off-diagonal pressure component, the 2nd of the two dimensions must be periodic.
   E.g. if the xy component is specified, then the y dimension must be periodic.

Cannot use fix nvt/npt/nph on a non-periodic dimension
   When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix nvt/npt/nph with both xy dynamics and xy scaling
   Self-explanatory.

Cannot use fix nvt/npt/nph with both xz dynamics and xz scaling
   Self-explanatory.

Cannot use fix nvt/npt/nph with both yz dynamics and yz scaling
   Self-explanatory.

Cannot use fix nvt/npt/nph with xy dynamics when y is non-periodic dimension
   The 2nd dimension in the barostatted tilt factor must be periodic.

Cannot use fix nvt/npt/nph with xz dynamics when z is non-periodic dimension
   The 2nd dimension in the barostatted tilt factor must be periodic.

Cannot use fix nvt/npt/nph with yz dynamics when z is non-periodic dimension
   The 2nd dimension in the barostatted tilt factor must be periodic.

Cannot use fix pour with triclinic box
   This feature is not yet supported.

Cannot use fix press/berendsen and fix deform on same component of stress tensor
   These commands both change the box size/shape, so you cannot use both together.
Cannot use fix press/berendsen on a non-periodic dimension
   Self-explanatory.
Cannot use fix press/berendsen with triclinic box
   Self-explanatory.
Cannot use fix reax/bonds without pair_style reax
   Self-explanatory.
Cannot use fix shake with non-molecular system
   Your choice of atom style does not have bonds.
Cannot use fix ttm with 2d simulation
   This is a current restriction of this fix due to the grid it creates.
Cannot use fix ttm with triclinic box
   This is a current restriction of this fix due to the grid it creates.
Cannot use fix wall in periodic dimension
   Self-explanatory.
Cannot use fix wall zlo/zhi for a 2d simulation
   Self-explanatory.
Cannot use fix wall/reflect in periodic dimension
   Self-explanatory.
Cannot use fix wall/reflect zlo/zhi for a 2d simulation
   Self-explanatory.
Cannot use fix wall/srd in periodic dimension
   Self-explanatory.
Cannot use fix wall/srd more than once
   Nor is there a need to since multiple walls can be specified in one command.
Cannot use fix wall/srd without fix srd
   Self-explanatory.
Cannot use fix wall/srd zlo/zhi for a 2d simulation
   Self-explanatory.
Cannot use force/hybrid_neigh with triclinic box
   Self-explanatory.
Cannot use force/neigh with triclinic box
   This is a current limitation of the GPU implementation in LAMMPS.
Cannot use kspace solver on system with no charge
   No atoms in system have a non-zero charge.
Cannot use lines with fix srd unless overlap is set
   This is because line segments are connected to each other.
Cannot use neigh_modify exclude with GPU neighbor builds
   This is a current limitation of the GPU implementation in LAMMPS.
Cannot use neighbor bins - box size << cutoff
   Too many neighbor bins will be created. This typically happens when the simulation box is very small in some dimension, compared to the neighbor cutoff. Use the "nsq" style instead of "bin" style.
Cannot use newton pair with buck/coul/cut/gpu pair style
   Self-explanatory.
Cannot use newton pair with buck/coul/long/gpu pair style
   Self-explanatory.
Cannot use newton pair with buck/gpu pair style
   Self-explanatory.
Cannot use newton pair with coul/long/gpu pair style
   Self-explanatory.
Cannot use newton pair with eam/gpu pair style
   Self-explanatory.
Cannot use newton pair with gayberne/gpu pair style
Cannot use newton pair with lj/charmm/coul/long/gpu pair style
   Self-explanatory.
Cannot use newton pair with lj/class2/coul/long/gpu pair style
   Self-explanatory.
Cannot use newton pair with lj/class2/gpu pair style
   Self-explanatory.
Cannot use newton pair with lj/cut/coul/cut/gpu pair style
   Self-explanatory.
Cannot use newton pair with lj/cut/coul/long/gpu pair style
   Self-explanatory.
Cannot use newton pair with lj/cut/gpu pair style
   Self-explanatory.
Cannot use newton pair with lj96/cut/gpu pair style
   Self-explanatory.
Cannot use newton pair with morse/gpu pair style
   Self-explanatory.
Cannot use newton pair with resquared/gpu pair style
   Self-explanatory.
Cannot use newton pair with table/gpu pair style
   Self-explanatory.
Cannot use newton pair with yukawa/gpu pair style
   Self-explanatory.
Cannot use non-zero forces in an energy minimization
   Fix setforce cannot be used in this manner. Use fix addforce instead.
Cannot use nonperiodic boundaries with fix ttm
   This fix requires a fully periodic simulation box.
Cannot use nonperiodic boundaries with Ewald
   For kspace style ewald, all 3 dimensions must have periodic boundaries unless you use the
   kspace_modify command to define a 2d slab with a non-periodic z dimension.
Cannot use nonperiodic boundaries with PPPM
   For kspace style pppm, all 3 dimensions must have periodic boundaries unless you use the kspace_modify
   command to define a 2d slab with a non-periodic z dimension.
Cannot use order greater than 8 with pppm/gpu.
   Self-explanatory.
Cannot use pair hybrid with GPU neighbor builds
   See documentation for fix gpu.
Cannot use pair tail corrections with 2d simulations
   The correction factors are only currently defined for 3d systems.
Cannot use processors part command without using partitions
   See the command-line -partition switch.
Cannot use ramp in variable formula between runs
   This is because the ramp() function is time dependent.
Cannot use region INF or EDGE when box does not exist
   Regions that extend to the box boundaries can only be used after the create_box command has been used.
Cannot use set atom with no atom IDs defined
   Atom IDs are not defined, so they cannot be used to identify an atom.
Cannot use set mol with no molecule IDs defined
   Self-explanatory.
Cannot use swiggle in variable formula between runs
This is a function of elapsed time.

*Cannot use tris with fix srd unless overlap is set*
This is because triangles are connected to each other.

*Cannot use variable energy with constant force in fix addforce*
This is because for constant force, LAMMPS can compute the change in energy directly.

*Cannot use variable every setting for dump dcd*
The format of DCD dump files requires snapshots be output at a constant frequency.

*Cannot use variable every setting for dump xtc*
The format of this file requires snapshots at regular intervals.

*Cannot use vdisplace in variable formula between runs*
This is a function of elapsed time.

*Cannot use velocity create loop all unless atoms have IDs*
Atoms in the simulation do not have IDs, so this style of velocity creation cannot be performed.

*Cannot use wall in periodic dimension*
Self-explanatory.

*Cannot wiggle and shear fix wall/gran*
Cannot specify both options at the same time.

*Cannot yet use fix balance with PPPM*
This is a current limitation of LAMMPS.

*Cannot zero Langevin force of 0 atoms*
The group has zero atoms, so you cannot request its force be zeroed.

*Cannot zero momentum of 0 atoms*
The collection of atoms for which momentum is being computed has no atoms.

*Change_box command before simulation box is defined*
Self-explanatory.

*Change_box volume used incorrectly*
The "dim volume" option must be used immediately following one or two settings for "dim1 ..." (and optionally "dim2 ...") and must be for a different dimension, i.e. dim ! = dim1 and dim ! = dim2.

*Communicate group ! = atom_modify first group*
Self-explanatory.

*Compute ID for compute atom/molecule does not exist*
Self-explanatory.

*Compute ID for compute reduce does not exist*
Self-explanatory.

*Compute ID for compute slice does not exist*
Self-explanatory.

*Compute ID for fix ave/atom does not exist*
Self-explanatory.

*Compute ID for fix ave/correlate does not exist*
Self-explanatory.

*Compute ID for fix ave/histo does not exist*
Self-explanatory.

*Compute ID for fix ave/spatial does not exist*
Self-explanatory.

*Compute ID for fix ave/time does not exist*
Self-explanatory.

*Compute ID for fix store/state does not exist*
Self-explanatory.

*Compute ID must be alphanumeric or underscore characters*
Self-explanatory.

*Compute angle/local used when angles are not allowed*
The atom style does not support angles.
Compute atom/molecule compute array is accessed out-of-range
   Self-explanatory.
Compute atom/molecule compute does not calculate a per-atom array
   Self-explanatory.
Compute atom/molecule compute does not calculate a per-atom vector
   Self-explanatory.
Compute atom/molecule compute does not calculate per-atom values
   Self-explanatory.
Compute atom/molecule fix array is accessed out-of-range
   Self-explanatory.
Compute atom/molecule fix does not calculate a per-atom array
   Self-explanatory.
Compute atom/molecule fix does not calculate a per-atom vector
   Self-explanatory.
Compute atom/molecule fix does not calculate per-atom values
   Self-explanatory.
Compute atom/molecule requires molecular atom style
   Self-explanatory.
Compute atom/molecule variable is not atom-style variable
   Self-explanatory.
Compute bond/local used when bonds are not allowed
   The atom style does not support bonds.
Compute centro/atom requires a pair style be defined
   This is because the computation of the centro-symmetry values uses a pairwise neighbor list.
Compute cluster/atom cutoff is longer than pairwise cutoff
   Cannot identify clusters beyond cutoff.
Compute cluster/atom requires a pair style be defined
   This is so that the pair style defines a cutoff distance which is used to find clusters.
Compute cna/atom cutoff is longer than pairwise cutoff
   Self-explanatory.
Compute cna/atom requires a pair style be defined
   Self-explanatory.
Compute com/molecule requires molecular atom style
   Self-explanatory.
Compute coord/atom cutoff is longer than pairwise cutoff
   Cannot compute coordination at distances longer than the pair cutoff, since those atoms are not in the
   neighbor list.
Compute coord/atom requires a pair style be defined
   Self-explanatory.
Compute damage/atom requires peridynamic potential
   Damage is a Peridynamic-specific metric. It requires you to be running a Peridynamics simulation.
Compute dihedral/local used when dihedrals are not allowed
   The atom style does not support dihedrals.
Compute does not allow an extra compute or fix to be reset
   This is an internal LAMMPS error. Please report it to the developers.
Compute erotate/asphere requires atom style ellipsoid or line or tri
   Self-explanatory.
Compute erotate/asphere requires extended particles
   This compute cannot be used with point paritlces.
Compute erotate/sphere requires atom style sphere
   Self-explanatory.
Compute event/displace has invalid fix event assigned
This is an internal LAMMPS error. Please report it to the developers.

Compute group/group group ID does not exist
Self-explanatory.

Compute gyration/molecule requires molecular atom style
Self-explanatory.

Compute heat/flux compute ID does not compute ke/atom
Self-explanatory.

Compute heat/flux compute ID does not compute pe/atom
Self-explanatory.

Compute heat/flux compute ID does not compute stress/atom
Self-explanatory.

Compute improper/local used when impropers are not allowed
The atom style does not support impropers.

Compute msd/molecule requires molecular atom style
Self-explanatory.

Compute nve/asphere requires atom style ellipsoid
Self-explanatory.

Compute nvt/nph/npt asphere requires atom style ellipsoid
Self-explanatory.

Compute pair must use group all
Pair styles accumulate energy on all atoms.

Compute pe must use group all
Energies computed by potentials (pair, bond, etc) are computed on all atoms.

Compute pressure must use group all
Virial contributions computed by potentials (pair, bond, etc) are computed on all atoms.

Compute pressure temperature ID does not compute temperature
The compute ID assigned to a pressure computation must compute temperature.

Compute property/atom for atom property that isn't allocated
Self-explanatory.

Compute property/local cannot use these inputs together
Only inputs that generate the same number of datums can be used together. E.g. bond and angle quantities cannot be mixed.

Compute property/local for property that isn't allocated
Self-explanatory.

Compute property/molecule requires molecular atom style
Self-explanatory.

Compute rdf requires a pair style be defined
Self-explanatory.

Compute reduce compute array is accessed out-of-range
An index for the array is out of bounds.

Compute reduce compute calculates global values
A compute that calculates peratom or local values is required.

Compute reduce compute does not calculate a local array
Self-explanatory.

Compute reduce compute does not calculate a local vector
Self-explanatory.

Compute reduce compute does not calculate a per-atom array
Self-explanatory.

Compute reduce compute does not calculate a per-atom vector
Self-explanatory.

Compute reduce fix array is accessed out-of-range
An index for the array is out of bounds.
Compute reduce fix calculates global values
   A fix that calculates peratom or local values is required.
Compute reduce fix does not calculate a local array
   Self-explanatory.
Compute reduce fix does not calculate a local vector
   Self-explanatory.
Compute reduce fix does not calculate a per-atom array
   Self-explanatory.
Compute reduce fix does not calculate a per-atom vector
   Self-explanatory.
Compute reduce replace requires min or max mode
   Self-explanatory.
Compute reduce variable is not atom-style variable
   Self-explanatory.
Compute slice compute array is accessed out-of-range
   An index for the array is out of bounds.
Compute slice compute does not calculate a global array
   Self-explanatory.
Compute slice compute does not calculate a global vector
   Self-explanatory.
Compute slice compute does not calculate global vector or array
   Self-explanatory.
Compute slice compute vector is accessed out-of-range
   The index for the vector is out of bounds.
Compute slice fix array is accessed out-of-range
   An index for the array is out of bounds.
Compute slice fix does not calculate a global array
   Self-explanatory.
Compute slice fix does not calculate a global vector
   Self-explanatory.
Compute slice fix does not calculate global vector or array
   Self-explanatory.
Compute slice fix vector is accessed out-of-range
   The index for the vector is out of bounds.
Compute temp/asphere requires atom style ellipsoid
   Self-explanatory.
Compute temp/asphere requires extended particles
   This compute cannot be used with point particles.
Compute temp/partial cannot use vz for 2d systems
   Self-explanatory.
Compute temp/profile cannot bin z for 2d systems
   Self-explanatory.
Compute temp/profile cannot use vz for 2d systems
   Self-explanatory.
Compute temp/sphere requires atom style sphere
   Self-explanatory.
Compute ti kspace style does not exist
   Self-explanatory.
Compute ti pair style does not exist
   Self-explanatory.
Compute ti tail when pair style does not compute tail corrections
   Self-explanatory.
Compute used in variable between runs is not current
Computes cannot be invoked by a variable in between runs. Thus they must have been evaluated on the last timestep of the previous run in order for their value(s) to be accessed. See the doc page for the variable command for more info.

Compute used in variable thermo keyword between runs is not current
Some thermo keywords rely on a compute to calculate their value(s). Computes cannot be invoked by a variable in between runs. Thus they must have been evaluated on the last timestep of the previous run in order for their value(s) to be accessed. See the doc page for the variable command for more info.

Computed temperature for fix temp/berendsen cannot be 0.0
Self-explanatory.

Computed temperature for fix temp/rescale cannot be 0.0
Cannot rescale the temperature to a new value if the current temperature is 0.0.

Could not count initial bonds in fix bond/create
Could not find one of the atoms in a bond on this processor.

Could not create 3d FFT plan
The FFT setup in pppm failed.

Could not create 3d grid of processors
The specified constraints did not allow a Px by Py by Pz grid to be created where Px * Py * Pz = P = total number of processors.

Could not create 3d remap plan
The FFT setup in pppm failed.

Could not create numa grid of processors
The specified constraints did not allow this style of grid to be created. Usually this is because the total processor count is not a multiple of the cores/node or the user specified processor count is > 1 in one of the dimensions.

Could not create twolevel 3d grid of processors
The specified constraints did not allow this style of grid to be created.

Could not find atom_modify first group ID
Self-explanatory.

Could not find change_box group ID
Group ID used in the change_box command does not exist.

Could not find compute ID for PRD
Self-explanatory.

Could not find compute ID for TAD
Self-explanatory.

Could not find compute ID for temperature bias
Self-explanatory.

Could not find compute ID to delete
Self-explanatory.

Could not find compute displace/atom fix ID
Self-explanatory.

Could not find compute event/displace fix ID
Self-explanatory.

Could not find compute group ID
Self-explanatory.

Could not find compute heat/flux compute ID
Self-explanatory.

Could not find compute msd fix ID
Self-explanatory.

Could not find compute pressure temperature ID
The compute ID for calculating temperature does not exist.

Could not find compute_modify ID
Self-explanatory.

Could not find delete_atoms group ID
Group ID used in the delete_atoms command does not exist.

Could not find delete_atoms region ID
Region ID used in the delete_atoms command does not exist.

Could not find displace_atoms group ID
Group ID used in the displace_atoms command does not exist.

Could not find dump custom compute ID
The compute ID needed by dump custom to compute a per-atom quantity does not exist.

Could not find dump custom fix ID
Self-explanatory.

Could not find dump custom variable name
Self-explanatory.

Could not find dump group ID
A group ID used in the dump command does not exist.

Could not find dump local compute ID
Self-explanatory.

Could not find dump local fix ID
Self-explanatory.

Could not find dump modify compute ID
Self-explanatory.

Could not find dump modify fix ID
Self-explanatory.

Could not find dump modify variable name
Self-explanatory.

Could not find fix ID to delete
Self-explanatory.

Could not find fix group ID
A group ID used in the fix command does not exist.

Could not find fix msst compute ID
Self-explanatory.

Could not find fix poems group ID
A group ID used in the fix poems command does not exist.

Could not find fix recenter group ID
A group ID used in the fix recenter command does not exist.

Could not find fix rigid group ID
A group ID used in the fix rigid command does not exist.

Could not find fix srd group ID
Self-explanatory.

Could not find fix_modify ID
A fix ID used in the fix_modify command does not exist.

Could not find fix_modify pressure ID
The compute ID for computing pressure does not exist.

Could not find fix_modify temperature ID
The compute ID for computing temperature does not exist.

Could not find group delete group ID
Self-explanatory.

Could not find set group ID
Group ID specified in set command does not exist.

Could not find thermo compute ID
Compute ID specified in thermo_style command does not exist.

Could not find thermo custom compute ID
The compute ID needed by thermo style custom to compute a requested quantity does not exist.

**Could not find thermo custom fix ID**

The fix ID needed by thermo style custom to compute a requested quantity does not exist.

**Could not find thermo custom variable name**

Self-explanatory.

**Could not find thermo fix ID**

Fix ID specified in thermo_style command does not exist.

**Could not find thermo variable name**

Self-explanatory.

**Could not find thermo_modify pressure ID**

The compute ID needed by thermo style custom to compute pressure does not exist.

**Could not find thermo_modify temperature ID**

The compute ID needed by thermo style custom to compute temperature does not exist.

**Could not find undump ID**

A dump ID used in the undump command does not exist.

**Could not find velocity group ID**

A group ID used in the velocity command does not exist.

**Could not find velocity temperature ID**

The compute ID needed by the velocity command to compute temperature does not exist.

**Could not find initialize a specified accelerator device**

Could not initialize at least one of the devices specified for the gpu package.

**Could not grab element entry from EIM potential file**

Self-explanatory.

**Could not grab global entry from EIM potential file**

Self-explanatory.

**Could not grab pair entry from EIM potential file**

Self-explanatory.

**Coulomb cutoffs of pair hybrid sub-styles do not match**

If using a Kspace solver, all Coulomb cutoffs of long pair styles must be the same.

**Could not find dump_modify ID**

Self-explanatory.

**Create_atoms command before simulation box is defined**

The create_atoms command cannot be used before a read_data, read_restart, or create_box command.

**Create_atoms region ID does not exist**

A region ID used in the create_atoms command does not exist.

**Create_box region ID does not exist**

A region ID used in the create_box command does not exist.

**Create_box region does not support a bounding box**

Not all regions represent bounded volumes. You cannot use such a region with the create_box command.

**Cyclic loop in joint connections**

Fix poems cannot (yet) work with coupled bodies whose joints connect the bodies in a ring (or cycle).

**Degenerate lattice primitive vectors**

Invalid set of 3 lattice vectors for lattice command.

**Delete region ID does not exist**

Self-explanatory.

**Delete_atoms command before simulation box is defined**

The delete_atoms command cannot be used before a read_data, read_restart, or create_box command.

**Delete_atoms cutoff > neighbor cutoff**

Cannot delete atoms further away than a processor knows about.

**Delete_atoms requires a pair style be defined**

This is because atom deletion within a cutoff uses a pairwise neighbor list.

**Delete_bonds command before simulation box is defined**
The delete_bonds command cannot be used before a read_data, read_restart, or create_box command.

Delete_bonds command with no atoms existing
No atoms are yet defined so the delete_bonds command cannot be used.

Deposition region extends outside simulation box
Self-explanatory.

Did not assign all atoms correctly
Atoms read in from a data file were not assigned correctly to processors. This is likely due to some atom coordinates being outside a non-periodic simulation box.

Did not find all elements in MEAM library file
The requested elements were not found in the MEAM file.

Did not find fix shake partner info
Could not find bond partners implied by fix shake command. This error can be triggered if the delete_bonds command was used before fix shake, and it removed bonds without resetting the 1-2, 1-3, 1-4 weighting list via the special keyword.

Did not find keyword in table file
Keyword used in pair_coeff command was not found in table file.

Did not set temp for fix rigid/nvt
The temp keyword must be used.

Dihedral atom missing in delete_bonds
The delete_bonds command cannot find one or more atoms in a particular dihedral on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid dihedral.

Dihedral atom missing in set command
The set command cannot find one or more atoms in a particular dihedral on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid dihedral.

Dihedral atoms %d %d %d %d missing on proc %d at step %ld
One or more of 4 atoms needed to compute a particular dihedral are missing on this processor. Typically this is because the pairwise cutoff is set too short or the dihedral has blown apart and an atom is too far away.

Dihedral charmm is incompatible with Pair style
Dihedral style charmm must be used with a pair style charmm in order for the 1-4 epsilon/sigma parameters to be defined.

Dihedral coeff for hybrid has invalid style
Dihedral style hybrid uses another dihedral style as one of its coefficients. The dihedral style used in the dihedral_coeff command or read from a restart file is not recognized.

Dihedral coeffs are not set
No dihedral coefficients have been assigned in the data file or via the dihedral_coeff command.

Dihedral style hybrid cannot have hybrid as an argument
Self-explanatory.

Dihedral style hybrid cannot have none as an argument
Self-explanatory.

Dihedral style hybrid cannot use same dihedral style twice
Self-explanatory.

Dihedral_coeff command before dihedral_style is defined
Coefficients cannot be set in the data file or via the dihedral_coeff command until an dihedral_style has been assigned.

Dihedral_coeff command before simulation box is defined
The dihedral_coeff command cannot be used before a read_data, read_restart, or create_box command.

Dihedral_coeff command when no dihedrals allowed
The chosen atom style does not allow for dihedrals to be defined.

Dihedral_style command when no dihedrals allowed
The chosen atom style does not allow for dihedrals to be defined.

Dihedrals assigned incorrectly
Dihedrals read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

**Dihedrals defined but no dihedral types**
The data file header lists dihedrals but no dihedral types.

**Dimension command after simulation box is defined**
The dimension command cannot be used after a read_data, read_restart, or create_box command.

**Displace_atoms command before simulation box is defined**
The displace_atoms command cannot be used before a read_data, read_restart, or create_box command.

**Distance must be > 0 for compute event/displace**
Self-explanatory.

**Divide by 0 in influence function of pair peri/lps**
This should not normally occur. It is likely a problem with your model.

**Divide by 0 in variable formula**
Self-explanatory.

**Domain too large for neighbor bins**
The domain has become extremely large so that neighbor bins cannot be used. Most likely, one or more atoms have been blown out of the simulation box to a great distance.

**Double precision is not supported on this accelerator**
Self-explanatory.

**Dump cfg arguments can not mix xs|ys|zs with xsu|ysu|zsu**
Self-explanatory.

**Dump cfg arguments must start with 'id type xs ys zs' or 'id type xsu ysu zsu'**
This is a requirement of the CFG output format.

**Dump cfg requires one snapshot per file**
Use the wildcard "*" character in the filename.

**Dump custom and fix not computed at compatible times**
The fix must produce per-atom quantities on timesteps that dump custom needs them.

**Dump custom compute does not calculate per-atom array**
Self-explanatory.

**Dump custom compute does not calculate per-atom vector**
Self-explanatory.

**Dump custom compute does not compute per-atom info**
Self-explanatory.

**Dump custom compute vector is accessed out-of-range**
Self-explanatory.

**Dump custom fix does not compute per-atom array**
Self-explanatory.

**Dump custom fix does not compute per-atom info**
Self-explanatory.

**Dump custom fix does not compute per-atom vector**
Self-explanatory.

**Dump custom fix vector is accessed out-of-range**
Self-explanatory.

**Dump custom variable is not atom-style variable**
Only atom-style variables generate per-atom quantities, needed for dump output.

**Dump dcd of non-matching # of atoms**
Every snapshot written by dump dcd must contain the same # of atoms.

**Dump dcd requires sorting by atom ID**
Use the dump_modify sort command to enable this.

**Dump every variable returned a bad timestep**
The variable must return a timestep greater than the current timestep.

**Dump file does not contain requested snapshot**
Dump file is incorrectly formatted
No atoms were found in file.

Dump image bond not allowed with no bond types
Self-explanatory.

Dump image cannot perform sorting
Self-explanatory.

Dump image persp option is not yet supported
Self-explanatory.

Dump image requires one snapshot per file
Use a "*" in the filename.

Dump local and fix not computed at compatible times
The fix must produce per-atom quantities on timesteps that dump local needs them.

Dump local attributes contain no compute or fix
Self-explanatory.

Dump local cannot sort by atom ID
This is because dump local does not really dump per-atom info.

Dump local compute does not calculate local array
Self-explanatory.

Dump local compute does not calculate local vector
Self-explanatory.

Dump local compute does not compute local info
Self-explanatory.

Dump local compute vector is accessed out-of-range
Self-explanatory.

Dump local count is not consistent across input fields
Every column of output must be the same length.

Dump local fix does not compute local array
Self-explanatory.

Dump local fix does not compute local info
Self-explanatory.

Dump local fix does not compute local vector
Self-explanatory.

Dump local fix vector is accessed out-of-range
Self-explanatory.

Dump modify bcolor not allowed with no bond types
Self-explanatory.

Dump modify bdiam not allowed with no bond types
Self-explanatory.

Dump modify compute ID does not compute per-atom array
Self-explanatory.

Dump modify compute ID does not compute per-atom info
Self-explanatory.

Dump modify compute ID does not compute per-atom vector
Self-explanatory.

Dump modify compute ID vector is not large enough
Self-explanatory.

Dump modify element names do not match atom types
Number of element names must equal number of atom types.

Dump modify fix ID does not compute per-atom array
Self-explanatory.

Dump modify fix ID does not compute per-atom info
Self-explanatory.

**Dump modify fix ID does not compute per-atom vector**
Self-explanatory.

**Dump modify fix ID vector is not large enough**
Self-explanatory.

**Dump modify variable is not atom-style variable**
Self-explanatory.

**Dump sort column is invalid**
Self-explanatory.

**Dump xtc requires sorting by atom ID**
Use the dump_modify sort command to enable this.

**Dump_modify region ID does not exist**
Self-explanatory.

**Dumping an atom property that isn't allocated**
The chosen atom style does not define the per-atom quantity being dumped.

**Dumping an atom quantity that isn't allocated**
Only per-atom quantities that are defined for the atom style being used are allowed.

**Duplicate fields in read_dump command**
Self-explanatory.

**Duplicate particle in PeriDynamic bond - simulation box is too small**
This is likely because your box length is shorter than 2 times the bond length.

**Electronic temperature dropped below zero**
Something has gone wrong with the fix ttm electron temperature model.

**Empty brackets in variable**
There is no variable syntax that uses empty brackets. Check the variable doc page.

**Energy was not tallied on needed timestep**
You are using a thermo keyword that requires potentials to have tallied energy, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

**Expected floating point parameter in input script or data file**
The quantity being read is an integer on non-numeric value.

**Expected floating point parameter in variable definition**
The quantity being read is a non-numeric value.

**Expected integer parameter in input script or data file**
The quantity being read is a floating point or non-numeric value.

**Expected integer parameter in variable definition**
The quantity being read is a floating point or non-numeric value.

**Failed to allocate %ld bytes for array %s**
Your LAMMPS simulation has run out of memory. You need to run a smaller simulation or on more processors.

**Failed to reallocate %ld bytes for array %s**
Your LAMMPS simulation has run out of memory. You need to run a smaller simulation or on more processors.

**Fewer SRD bins than processors in some dimension**
This is not allowed. Make your SRD bin size smaller.

**Final box dimension due to fix deform is < 0.0**
Self-explanatory.

**Fix GCMC incompatible with given pair_style**
Some pair_styles do not provide single-atom energies, which are needed by fix GCMC.

**Fix GCMC molecule command requires atom attribute molecule**
Should not choose the GCMC molecule feature if no molecules are being simulated. The general molecule flag is off, but GCMC's molecule flag is on.

**Fix GCMC molecule feature does not yet work**
Fix GCMC cannot (yet) be used to exchange molecules, only atoms.

Fix GPU split must be positive for hybrid pair styles
Self-explanatory.

Fix ID for compute atom/molecule does not exist
Self-explanatory.

Fix ID for compute reduce does not exist
Self-explanatory.

Fix ID for compute slice does not exist
Self-explanatory.

Fix ID for fix ave/atom does not exist
Self-explanatory.

Fix ID for fix ave/correlate does not exist
Self-explanatory.

Fix ID for fix ave/histo does not exist
Self-explanatory.

Fix ID for fix ave/spatial does not exist
Self-explanatory.

Fix ID for fix ave/time does not exist
Self-explanatory.

Fix ID for fix store/state does not exist
Self-explanatory.

Fix ID for read_data does not exist
Self-explanatory.

Fix ID must be alphanumeric or underscore characters
Self-explanatory.

Fix SRD no-slip requires atom attribute torque
This is because the SRD collisions will impart torque to the solute particles.

Fix SRD: bad bin assignment for SRD advection
Something has gone wrong in your SRD model; try using more conservative settings.

Fix SRD: bad search bin assignment
Something has gone wrong in your SRD model; try using more conservative settings.

Fix SRD: bad stencil bin for big particle
Something has gone wrong in your SRD model; try using more conservative settings.

Fix SRD: too many big particles in bin
Reset the ATOMPERBIN parameter at the top of fix_srd.cpp to a larger value, and re-compile the code.

Fix SRD: too many walls in bin
This should not happen unless your system has been setup incorrectly.

Fix adapt kspace style does not exist
Self-explanatory.

Fix adapt pair style does not exist
Self-explanatory

Fix adapt pair style param not supported
The pair style does not know about the parameter you specified.

Fix adapt requires atom attribute diameter
The atom style being used does not specify an atom diameter.

Fix adapt type pair range is not valid for pair hybrid sub-style
Self-explanatory.

Fix ave/atom compute array is accessed out-of-range
Self-explanatory.

Fix ave/atom compute does not calculate a per-atom array
Self-explanatory.

Fix ave/atom compute does not calculate a per-atom vector
A compute used by fix ave/atom must generate per-atom values.

Fix ave/atom compute does not calculate per-atom values
A compute used by fix ave/atom must generate per-atom values.

Fix ave/atom fix array is accessed out-of-range
Self-explanatory.

Fix ave/atom fix does not calculate a per-atom array
Self-explanatory.

Fix ave/atom fix does not calculate a per-atom vector
A fix used by fix ave/atom must generate per-atom values.

Fix ave/atom fix does not calculate per-atom values
A fix used by fix ave/atom must generate per-atom values.

Fix ave/atom missed timestep
You cannot reset the timestep to a value beyond where the fix expects to next perform averaging.

Fix ave/atom variable is not atom-style variable
A variable used by fix ave/atom must generate per-atom values.

Fix ave/correlate compute does not calculate a scalar
Self-explanatory.

Fix ave/correlate compute does not calculate a vector
Self-explanatory.

Fix ave/correlate compute vector is accessed out-of-range
The index for the vector is out of bounds.

Fix ave/correlate fix does not calculate a scalar
Self-explanatory.

Fix ave/correlate fix does not calculate a vector
Self-explanatory.

Fix ave/correlate fix vector is accessed out-of-range
The index for the vector is out of bounds.

Fix ave/correlate missed timestep
You cannot reset the timestep to a value beyond where the fix expects to next perform averaging.

Fix ave/correlate variable is not equal-style variable
Self-explanatory.

Fix ave/histo cannot input local values in scalar mode
Self-explanatory.

Fix ave/histo cannot input per-atom values in scalar mode
Self-explanatory.

Fix ave/histo compute array is accessed out-of-range
Self-explanatory.

Fix ave/histo compute does not calculate a global array
Self-explanatory.

Fix ave/histo compute does not calculate a global scalar
Self-explanatory.

Fix ave/histo compute does not calculate a global vector
Self-explanatory.

Fix ave/histo compute does not calculate a local array
Self-explanatory.

Fix ave/histo compute does not calculate a local vector
Self-explanatory.

Fix ave/histo compute does not calculate a per-atom array
Self-explanatory.

Fix ave/histo compute does not calculate a per-atom vector
Self-explanatory.

Fix ave/histo compute does not calculate local values
Self-explanatory.

Fix ave/histo compute does not calculate per-atom values
Self-explanatory.

Fix ave/histo compute vector is accessed out-of-range
Self-explanatory.

Fix ave/histo fix array is accessed out-of-range
Self-explanatory.

Fix ave/histo fix does not calculate a global array
Self-explanatory.

Fix ave/histo fix does not calculate a global scalar
Self-explanatory.

Fix ave/histo fix does not calculate a global vector
Self-explanatory.

Fix ave/histo fix does not calculate a local array
Self-explanatory.

Fix ave/histo fix does not calculate a local vector
Self-explanatory.

Fix ave/histo fix does not calculate a per-atom array
Self-explanatory.

Fix ave/histo fix does not calculate a per-atom vector
Self-explanatory.

Fix ave/histo fix does not calculate local values
Self-explanatory.

Fix ave/histo fix does not calculate per-atom values
Self-explanatory.

Fix ave/histo fix vector is accessed out-of-range
Self-explanatory.

Fix ave/histo input is invalid compute
Self-explanatory.

Fix ave/histo input is invalid fix
Self-explanatory.

Fix ave/histo input is invalid variable
Self-explanatory.

Fix ave/histo inputs are not all global, peratom, or local
All inputs in a single fix ave/histo command must be of the same style.

Fix ave/histo missed timestep
You cannot reset the timestep to a value beyond where the fix expects to next perform averaging.

Fix ave/spatial compute does not calculate a per-atom array
Self-explanatory.

Fix ave/spatial compute does not calculate a per-atom vector
A compute used by fix ave/spatial must generate per-atom values.

Fix ave/spatial compute does not calculate per-atom values
A compute used by fix ave/spatial must generate per-atom values.

Fix ave/spatial compute vector is accessed out-of-range
The index for the vector is out of bounds.

Fix ave/spatial fix does not calculate a per-atom array
Self-explanatory.

Fix ave/spatial fix does not calculate a per-atom vector
A fix used by fix ave/spatial must generate per-atom values.

Fix ave/spatial fix does not calculate per-atom values
A fix used by fix ave/spatial must generate per-atom values.

Fix ave/spatial fix vector is accessed out-of-range
The index for the vector is out of bounds.

Fix ave/spatial for triclinic boxes requires units reduced
Self-explanatory.

Fix ave/spatial missed timestep
You cannot reset the timestep to a value beyond where the fix expects to next perform averaging.

Fix ave/spatial settings invalid with changing box
If the ave setting is "running" or "window" and the box size/shape changes during the simulation, then the units setting must be "reduced", else the number of bins may change.

Fix ave/spatial variable is not atom-style variable
A variable used by fix ave/spatial must generate per-atom values.

Fix ave/time cannot set output array intensive/extensive from these inputs
One of more of the vector inputs has individual elements which are flagged as intensive or extensive.
Such an input cannot be flagged as all intensive/extensive when turned into an array by fix ave/time.

Fix ave/time cannot use variable with vector mode
Variables produce scalar values.

Fix ave/time columns are inconsistent lengths
Self-explanatory.

Fix ave/time compute array is accessed out-of-range
An index for the array is out of bounds.

Fix ave/time compute does not calculate a scalar
Self-explanatory.

Fix ave/time compute does not calculate a vector
Self-explanatory.

Fix ave/time compute does not calculate an array
Self-explanatory.

Fix ave/time compute vector is accessed out-of-range
The index for the vector is out of bounds.

Fix ave/time fix array is accessed out-of-range
An index for the array is out of bounds.

Fix ave/time fix does not calculate a scalar
Self-explanatory.

Fix ave/time fix does not calculate a vector
Self-explanatory.

Fix ave/time fix does not calculate an array
Self-explanatory.

Fix ave/time fix vector is accessed out-of-range
The index for the vector is out of bounds.

Fix ave/time missed timestep
You cannot reset the timestep to a value beyond where the fix expects to next perform averaging.

Fix ave/time variable is not equal-style variable
Self-explanatory.

Fix balance string is invalid
The string can only contain the characters "x", "y", or "z".

Fix balance string is invalid for 2d simulation
The string cannot contain the letter "z".

Fix bond/break requires special_bonds = 0,1,1
This is a restriction of the current fix bond/break implementation.

Fix bond/create cutoff is longer than pairwise cutoff
This is not allowed because bond creation is done using the pairwise neighbor list.

Fix bond/create requires special_bonds coul = 0,1,1
Self-explanatory.

Fix bond/create requires special_bonds lj = 0,1,1
Self-explanatory.

Fix bond/swap cannot use dihedral or improper styles
These styles cannot be defined when using this fix.
Fix bond/swap requires pair and bond styles
Self-explanatory.
Fix bond/swap requires special_bonds = 0,1,1
Self-explanatory.
Fix box/relax generated negative box length
The pressure being applied is likely too large. Try applying it incrementally, to build to the high pressure.
Fix command before simulation box is defined
The fix command cannot be used before a read_data, read_restart, or create_box command.
Fix deform cannot use xy variable with yz
The yz setting cannot be a variable if xy deformation is also specified. This is because LAMMPS cannot determine if the yz setting will induce a box flip which would be invalid if xy is also changing.
Fix deform is changing yz too much with xy
When both yz and xy are changing, it induces changes in xz if the box must flip from one tilt extreme to another. Thus it is not allowed for yz to grow so much that a flip is induced.
Fix deform tilt factors require triclinic box
Cannot deform the tilt factors of a simulation box unless it is a triclinic (non-orthogonal) box.
Fix deform volume setting is invalid
Cannot use volume style unless other dimensions are being controlled.
Fix deposit region cannot be dynamic
Only static regions can be used with fix deposit.
Fix deposit region does not support a bounding box
Not all regions represent bounded volumes. You cannot use such a region with the fix deposit command.
Fix efield requires atom attribute q
Self-explanatory.
Fix evaporate molecule requires atom attribute molecule
The atom style being used does not define a molecule ID.
Fix external callback function not set
This must be done by an external program in order to use this fix.
Fix for fix ave/atom not computed at compatible time
Fixes generate their values on specific timesteps. Fix ave/atom is requesting a value on a non-allowed timestep.
Fix for fix ave/correlate not computed at compatible time
Fixes generate their values on specific timesteps. Fix ave/correlate is requesting a value on a non-allowed timestep.
Fix for fix ave/histo not computed at compatible time
Fixes generate their values on specific timesteps. Fix ave/histo is requesting a value on a non-allowed timestep.
Fix for fix ave/spatial not computed at compatible time
Fixes generate their values on specific timesteps. Fix ave/spatial is requesting a value on a non-allowed timestep.
Fix for fix ave/time not computed at compatible time
Fixes generate their values on specific timesteps. Fix ave/time is requesting a value on a non-allowed timestep.
Fix for fix store/state not computed at compatible time
Fixes generate their values on specific timesteps. Fix store/state is requesting a value on a non-allowed timestep.
Fix freeze requires atom attribute torque
The atom style defined does not have this attribute.
Fix heat group has no atoms
Fix *heat kinetic energy went negative*
This will cause the velocity rescaling about to be performed by fix heat to be invalid.

Fix *in variable not computed at compatible time*
Fixes generate their values on specific timesteps. The variable is requesting the values on a non-allowed timestep.

Fix *langevin angmom requires atom style ellipsoid*
Self-explanatory.

Fix *langevin angmom requires extended particles*
This fix option cannot be used with point particles.

Fix *langevin omega requires atom style sphere*
Self-explanatory.

Fix *langevin omega requires extended particles*
One of the particles has radius 0.0.

Fix *langevin period must be > 0.0*
The time window for temperature relaxation must be > 0

Fix *langevin variable returned negative temperature*
Self-explanatory.

Fix *momentum group has no atoms*
Self-explanatory.

Fix *move cannot define z or vz variable for 2d problem*
Self-explanatory.

Fix *move cannot have 0 length rotation vector*
Self-explanatory.

Fix *move cannot rotate around non z-axis for 2d problem*
Self-explanatory.

Fix *move cannot set linear z motion for 2d problem*
Self-explanatory.

Fix *move cannot set wiggle z motion for 2d problem*
Self-explanatory.

Fix *msst compute ID does not compute potential energy*
Self-explanatory.

Fix *msst compute ID does not compute pressure*
Self-explanatory.

Fix *msst compute ID does not compute temperature*
Self-explanatory.

Fix *msst requires a periodic box*
Self-explanatory.

Fix *msst tscale must satisfy 0 <= tscale < 1*
Self-explanatory.

Fix *npt/nph has tilted box too far in one step - periodic cell is too far from equilibrium state*
Self-explanatory. The change in the box tilt is too extreme on a short timescale.

Fix *nve/asphere requires extended particles*
This fix can only be used for particles with a shape setting.

Fix *nve/asphere/noforce requires atom style ellipsoid*
Self-explanatory.

Fix *nve/asphere/noforce requires extended particles*
One of the particles is not an ellipsoid.

Fix *nve/line can only be used for 2d simulations*
Self-explanatory.

Fix *nve/line requires atom style line*
Self-explanatory.
Fix nve/line requires line particles
   Self-explanatory.
Fix nve/sphere requires atom attribute mu
   An atom style with this attribute is needed.
Fix nve/sphere requires atom style sphere
   Self-explanatory.
Fix nve/sphere requires extended particles
   This fix can only be used for particles of a finite size.
Fix nve/tri can only be used for 3d simulations
   Self-explanatory.
Fix nve/tri requires atom style tri
   Self-explanatory.
Fix nve/tri requires tri particles
   Self-explanatory.
Fix nvt/nph/npt asphere requires extended particles
   The shape setting for a particle in the fix group has shape = 0.0, which means it is a point particle.
Fix nvt/nph/npt sphere requires atom style sphere
   Self-explanatory.
Fix nvt/nph/npt damping parameters must be > 0.0
   Self-explanatory.
Fix nvt/nph/npt dilate group ID does not exist
   Self-explanatory.
Fix nvt/sphere requires extended particles
   This fix can only be used for particles of a finite size.
Fix orient/fcc file open failed
   The fix orient/fcc command could not open a specified file.
Fix orient/fcc file read failed
   The fix orient/fcc command could not read the needed parameters from a specified file.
Fix orient/fcc found self twice
   The neighbor lists used by fix orient/fcc are messed up. If this error occurs, it is likely a bug, so send an
   email to the developers.
Fix peri neigh does not exist
   Somehow a fix that the pair style defines has been deleted.
Fix pour region ID does not exist
   Self-explanatory.
Fix pour region cannot be dynamic
   Only static regions can be used with fix pour.
Fix pour region does not support a bounding box
   Not all regions represent bounded volumes. You cannot use such a region with the fix pour command.
Fix pour requires atom attributes radius, rmass
   The atom style defined does not have these attributes.
Fix press/berendsen damping parameters must be > 0.0
   Self-explanatory.
Fix qeq/comb group has no atoms
   Self-explanatory.
Fix qeq/comb requires atom attribute q
   An atom style with charge must be used to perform charge equilibration.
Fix reax/bonds numbonds > nsbmax_most
   The limit of the number of bonds expected by the ReaxFF force field was exceeded.
Fix recenter group has no atoms
   Self-explanatory.
Fix restrain requires an atom map, see atom_modify
Fix rigid atom has non-zero image flag in a non-periodic dimension
You cannot set image flags for non-periodic dimensions.

Fix rigid langevin period must be > 0.0
Self-explanatory.

Fix rigid molecule requires atom attribute molecule
Self-explanatory.

Fix rigid xy torque cannot be on for 2d simulation
Self-explanatory.

Fix rigid z force cannot be on for 2d simulation
Self-explanatory.

Fix rigid/nvt period must be > 0.0
Self-explanatory

Fix rigid: Bad principal moments
The principal moments of inertia computed for a rigid body are not within the required tolerances.

Fix shake cannot be used with minimization
Cannot use fix shake while doing an energy minimization since it turns off bonds that should contribute to the energy.

Fix spring couple group ID does not exist
Self-explanatory.

Fix srd lambda must be >= 0.6 of SRD grid size
This is a requirement for accuracy reasons.

Fix srd requires SRD particles all have same mass
Self-explanatory.

Fix srd requires ghost atoms store velocity
Use the communicate vel yes command to enable this.

Fix srd requires newton pair on
Self-explanatory.

Fix store/state compute array is accessed out-of-range
Self-explanatory.

Fix store/state compute does not calculate a per-atom array
The compute calculates a per-atom vector.

Fix store/state compute does not calculate a per-atom vector
The compute calculates a per-atom vector.

Fix store/state compute does not calculate per-atom values
Computes that calculate global or local quantities cannot be used with fix store/state.

Fix store/state fix array is accessed out-of-range
Self-explanatory.

Fix store/state fix does not calculate a per-atom array
The fix calculates a per-atom vector.

Fix store/state fix does not calculate a per-atom vector
The fix calculates a per-atom array.

Fix store/state fix does not calculate per-atom values
Fixes that calculate global or local quantities cannot be used with fix store/state.

Fix store/state for atom property that isn’t allocated
Self-explanatory.

Fix store/state variable is not atom-style variable
Only atom-style variables calculate per-atom quantities.

Fix temp/berendsen period must be > 0.0
Self-explanatory.

Fix temp/berendsen variable returned negative temperature
Self-explanatory.
Fix temp/rescale variable returned negative temperature
  Self-explanatory.
Fix thermal/conductivity swap value must be positive
  Self-explanatory.
Fix tmd must come after integration fixes
  Any fix tmd command must appear in the input script after all time integration fixes (nve, nvt, npt). See
  the fix tmd documentation for details.
Fix ttm electron temperatures must be > 0.0
  Self-explanatory.
Fix ttm electronic_density must be > 0.0
  Self-explanatory.
Fix ttm electronic_specific_heat must be > 0.0
  Self-explanatory.
Fix ttm electronic_thermal_conductivity must be >= 0.0
  Self-explanatory.
Fix ttm gamma_p must be > 0.0
  Self-explanatory.
Fix ttm gamma_s must be >= 0.0
  Self-explanatory.
Fix ttm number of nodes must be > 0
  Self-explanatory.
Fix ttm v_0 must be >= 0.0
  Self-explanatory.
Fix used in compute atom/molecule not computed at compatible time
  The fix must produce per-atom quantities on timesteps that the compute needs them.
Fix used in compute reduce not computed at compatible time
  Fixes generate their values on specific timesteps. Compute reduce is requesting a value on a non-allowed
timestep.
Fix used in compute slice not computed at compatible time
  Fixes generate their values on specific timesteps. Compute slice is requesting a value on a non-allowed
timestep.
Fix viscosity swap value must be positive
  Self-explanatory.
Fix viscosity vtarget value must be positive
  Self-explanatory.
Fix wall cutoff <= 0.0
  Self-explanatory.
Fix wall/colloid requires atom style sphere
  Self-explanatory.
Fix wall/colloid requires extended particles
  One of the particles has radius 0.0.
Fix wall/gran is incompatible with Pair style
  Must use a granular pair style to define the parameters needed for this fix.
Fix wall/gran requires atom style sphere
  Self-explanatory.
Fix wall/piston command only available at zlo
  The face keyword must be zlo.
Fix wall/region colloid requires atom style sphere
  Self-explanatory.
Fix wall/region colloid requires extended particles
  One of the particles has radius 0.0.
Fix wall/region cutoff <= 0.0
Self-explanatory.

**Fix modify order must be 3 or 5**
Self-explanatory.

**Fix modify pressure ID does not compute pressure**
The compute ID assigned to the fix must compute pressure.

**Fix modify temperature ID does not compute temperature**
The compute ID assigned to the fix must compute temperature.

**For triclinic deformation, specified target stress must be hydrostatic**
Triclinic pressure control is allowed using the tri keyword, but non-hydrostatic pressure control cannot be used in this case.

**Found no restart file matching pattern**
When using a "*" in the restart file name, no matching file was found.

**GPU library not compiled for this accelerator**
Self-explanatory.

**GPU particle split must be set to 1 for this pair style.**
For this pair style, you cannot run part of the force calculation on the host. See the package command.

**Gmask function in equal-style variable formula**
Gmask is per-atom operation.

**Gravity changed since fix pour was created**
Gravity must be static and not dynamic for use with fix pour.

**Gravity must point in -y to use with fix pour in 2d**
Gravity must be pointing "down" in a 2d box.

**Gravity must point in -z to use with fix pour in 3d**
Gravity must be pointing "down" in a 3d box, i.e. theta = 180.0.

**Grmask function in equal-style variable formula**
Grmask is per-atom operation.

**Group ID does not exist**
A group ID used in the group command does not exist.

**Group ID in variable formula does not exist**
Self-explanatory.

**Group command before simulation box is defined**
The group command cannot be used before a read_data, read_restart, or create_box command.

**Group region ID does not exist**
A region ID used in the group command does not exist.

**If read_dump purges it cannot replace or trim**
These operations are not compatible. See the read_dump doc page for details.

**Illegal ... command**
Self-explanatory. Check the input script syntax and compare to the documentation for the command. You can use -echo screen as a command-line option when running LAMMPS to see the offending line.

**Illegal COMB parameter**
One or more of the coefficients defined in the potential file is invalid.

**Illegal Stillinger-Weber parameter**
One or more of the coefficients defined in the potential file is invalid.

**Illegal Tersoff parameter**
One or more of the coefficients defined in the potential file is invalid.

**Illegal fix wall/piston velocity**
The piston velocity must be positive.

**Illegal integrate style**
Self-explanatory.

**Illegal number of angle table entries**
There must be at least 2 table entries.

**Illegal number of bond table entries**
There must be at least 2 table entries.

*Illegal number of pair table entries*

There must be at least 2 table entries.

*Illegal simulation box*

The lower bound of the simulation box is greater than the upper bound.

*Improper atom missing in delete_bonds*

The delete_bonds command cannot find one or more atoms in a particular improper on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid improper.

*Improper atom missing in set command*

The set command cannot find one or more atoms in a particular improper on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid improper.

*Improper atoms %d %d %d %d missing on proc %d at step %ld*

One or more of 4 atoms needed to compute a particular improper are missing on this processor. Typically this is because the pairwise cutoff is set too short or the improper has blown apart and an atom is too far away.

*Improper coeff for hybrid has invalid style*

Improper style hybrid uses another improper style as one of its coefficients. The improper style used in the improper_coeff command or read from a restart file is not recognized.

*Improper coeffs are not set*

No improper coefficients have been assigned in the data file or via the improper_coeff command.

*Improper style hybrid cannot have hybrid as an argument*

Self-explanatory.

*Improper style hybrid cannot have none as an argument*

Self-explanatory.

*Improper style hybrid cannot use same improper style twice*

Self-explanatory.

*Improper_coeff command before improper_style is defined*

Coefficients cannot be set in the data file or via the improper_coeff command until an improper_style has been assigned.

*Improper_coeff command before simulation box is defined*

The improper_coeff command cannot be used before a read_data, read_restart, or create_box command.

*Improper_coeff command when no impropers allowed*

The chosen atom style does not allow for impropers to be defined.

*Improper_style command when no impropers allowed*

The chosen atom style does not allow for impropers to be defined.

*Impropers assigned incorrectly*

Impropers read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

*Impropers defined but no improper types*

The data file header lists improper but no improper types.

*Inconsistent iparam/jparam values in fix bond/create command*

If itype and jtype are the same, then their maxbond and newtype settings must also be the same.

*Inconsistent line segment in data file*

The end points of the line segment are not equal distances from the center point which is the atom coordinate.

*Inconsistent triangle in data file*

The centroid of the triangle as defined by the corner points is not the atom coordinate.

*Incorrect args for angle coefficients*

Self-explanatory. Check the input script or data file.

*Incorrect args for bond coefficients*

Self-explanatory. Check the input script or data file.

*Incorrect args for dihedral coefficients*
Self-explanatory. Check the input script or data file.

Incorrect args for improper coefficients
Self-explanatory. Check the input script or data file.

Incorrect args for pair coefficients
Self-explanatory. Check the input script or data file.

Incorrect args in pair_style command
Self-explanatory.

Incorrect atom format in data file
Number of values per atom line in the data file is not consistent with the atom style.

Incorrect bonus data format in data file
See the read_data doc page for a description of how various kinds of bonus data must be formatted for certain atom styles.

Incorrect boundaries with slab Ewald
Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with Ewald.

Incorrect boundaries with slab PPPM
Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with PPPM.

Incorrect element names in ADP potential file
The element names in the ADP file do not match those requested.

Incorrect element names in EAM potential file
The element names in the EAM file do not match those requested.

Incorrect format in COMB potential file
Incorrect number of words per line in the potential file.

Incorrect format in MEAM potential file
Incorrect number of words per line in the potential file.

Incorrect format in NEB coordinate file
Self-explanatory.

Incorrect format in Stillinger-Weber potential file
Incorrect number of words per line in the potential file.

Incorrect format in TMD target file
Format of file read by fix tmd command is incorrect.

Incorrect format in Tersoff potential file
Incorrect number of words per line in the potential file.

Incorrect multiplicity arg for dihedral coefficients
Self-explanatory. Check the input script or data file.

Incorrect rigid body format in fix rigid file
The number of fields per line is not what expected.

Incorrect sign arg for dihedral coefficients
Self-explanatory. Check the input script or data file.

Incorrect velocity format in data file
Each atom style defines a format for the Velocity section of the data file. The read-in lines do not match.

Incorrect weight arg for dihedral coefficients
Self-explanatory. Check the input script or data file.

Index between variable brackets must be positive
Self-explanatory.

Indexed per-atom vector in variable formula without atom map
Accessing a value from an atom vector requires the ability to lookup an atom index, which is provided by an atom map. An atom map does not exist (by default) for non-molecular problems. Using the atom_modify map command will force an atom map to be created.

Initial temperatures not all set in fix ttm
Self-explanatory.

Input line quote not followed by whitespace
An end quote must be followed by whitespace.
Input line too long after variable substitution
   This is a hard (very large) limit defined in the input.cpp file.
Input line too long: %s
   This is a hard (very large) limit defined in the input.cpp file.
Insertion region extends outside simulation box
   Region specified with fix pour command extends outside the global simulation box.
Insufficient Jacobi rotations for POEMS body
   Eigensolve for rigid body was not sufficiently accurate.
Insufficient Jacobi rotations for rigid body
   Eigensolve for rigid body was not sufficiently accurate.
Insufficient Jacobi rotations for triangle
   The calculation of the inertia tensor of the triangle failed. This should not happen if it is a reasonably shaped triangle.
Insufficient memory on accelerator
   There is insufficient memory on one of the devices specified for the gpu package
Invalid -reorder N value
   Self-explanatory.
Invalid Boolean syntax in if command
   Self-explanatory.
Invalid REAX atom type
   There is a mis-match between LAMMPS atom types and the elements listed in the ReaxFF force field file.
Invalid angle style
   The choice of angle style is unknown.
Invalid angle table length
   Length must be 2 or greater.
Invalid angle type in Angles section of data file
   Angle type must be positive integer and within range of specified angle types.
Invalid angle type index for fix shake
   Self-explanatory.
Invalid atom ID in Angles section of data file
   Atom IDs must be positive integers and within range of defined atoms.
Invalid atom ID in Atoms section of data file
   Atom IDs must be positive integers.
Invalid atom ID in Bonds section of data file
   Atom IDs must be positive integers and within range of defined atoms.
Invalid atom ID in Bonus section of data file
   Atom IDs must be positive integers and within range of defined atoms.
Invalid atom ID in Dihedrals section of data file
   Atom IDs must be positive integers and within range of defined atoms.
Invalid atom ID in Impropers section of data file
   Atom IDs must be positive integers and within range of defined atoms.
Invalid atom ID in Velocities section of data file
   Atom IDs must be positive integers and within range of defined atoms.
Invalid atom mass for fix shake
   Mass specified in fix shake command must be > 0.0.
Invalid atom style
   The choice of atom style is unknown.
Invalid atom type in Atoms section of data file
   Atom types must range from 1 to specified # of types.
Invalid atom type in create_atoms command
   The create_box command specified the range of valid atom types. An invalid type is being requested.
Invalid atom type in fix GCMC command
   The atom type specified in the GCMC command does not exist.
Invalid atom type in fix bond/create command
   Self-explanatory.
Invalid atom type in neighbor exclusion list
   Atom types must range from 1 to Ntypes inclusive.
Invalid atom type index for fix shake
   Atom types must range from 1 to Ntypes inclusive.
Invalid atom types in pair_write command
   Atom types must range from 1 to Ntypes inclusive.
Invalid atom vector in variable formula
   The atom vector is not recognized.
Invalid attribute in dump custom command
   Self-explanatory.
Invalid attribute in dump local command
   Self-explanatory.
Invalid attribute in dump modify command
   Self-explanatory.
Invalid bond style
   The choice of bond style is unknown.
Invalid bond table length
   Length must be 2 or greater.
Invalid bond type in Bonds section of data file
   Bond type must be positive integer and within range of specified bond types.
Invalid bond type in fix bond/break command
   Self-explanatory.
Invalid bond type in fix bond/create command
   Self-explanatory.
Invalid bond type index for fix shake
   Self-explanatory. Check the fix shake command in the input script.
Invalid coeffs for this dihedral style
   Cannot set class 2 coeffs in data file for this dihedral style.
Invalid color in dump_modify command
   The specified color name was not in the list of recognized colors. See the dump_modify doc page.
Invalid command-line argument
   One or more command-line arguments is invalid. Check the syntax of the command you are using to launch LAMMPS.
Invalid compute ID in variable formula
   The compute is not recognized.
Invalid compute style
   Self-explanatory.
Invalid cutoff in communicate command
   Specified cutoff must be >= 0.0.
Invalid cutoffs in pair_write command
   Inner cutoff must be larger than 0.0 and less than outer cutoff.
Invalid d1 or d2 value for pair colloid coeff
   Neither d1 or d2 can be < 0.
Invalid data file section: Angle Coeffs
   Atom style does not allow angles.
Invalid data file section: AngleAngle Coeffs
   Atom style does not allow impropers.
Invalid data file section: AngleAngleTorsion Coeffs
Atom style does not allow dihedrals.  
*Invalid data file section: AngleTorsion Coeffs*  
Atom style does not allow dihedrals.  
*Invalid data file section: Angles*  
Atom style does not allow angles.  
*Invalid data file section: Bond Coeffs*  
Atom style does not allow bonds.  
*Invalid data file section: BondAngle Coeffs*  
Atom style does not allow angles.  
*Invalid data file section: BondBond Coeffs*  
Atom style does not allow angles.  
*Invalid data file section: BondBond13 Coeffs*  
Atom style does not allow dihedrals.  
*Invalid data file section: Bonds*  
Atom style does not allow bonds.  
*Invalid data file section: Dihedral Coeffs*  
Atom style does not allow dihedrals.  
*Invalid data file section: Dihedrals*  
Atom style does not allow dihedrals.  
*Invalid data file section: Ellipsoids*  
Atom style does not allow ellipsoids.  
*Invalid data file section: EndBondTorsion Coeffs*  
Atom style does not allow dihedrals.  
*Invalid data file section: Improper Coeffs*  
Atom style does not allow impropers.  
*Invalid data file section: Impropers*  
Atom style does not allow impropers.  
*Invalid data file section: Lines*  
Atom style does not allow lines.  
*Invalid data file section: MiddleBondTorsion Coeffs*  
Atom style does not allow dihedrals.  
*Invalid data file section: Triangles*  
Atom style does not allow triangles.  
*Invalid delta_conf in tad command*  
The value must be between 0 and 1 inclusive.  
*Invalid density in Atoms section of data file*  
Density value cannot be <= 0.0.  
*Invalid diameter in set command*  
Self-explanatory.  
*Invalid dihedral style*  
The choice of dihedral style is unknown.  
*Invalid dihedral type in Dihedrals section of data file*  
Dihedral type must be positive integer and within range of specified dihedral types.  
*Invalid dipole length in set command*  
Self-explanatory.  
*Invalid dump dcd filename*  
Filenames used with the dump dcd style cannot be binary or compressed or cause multiple files to be written.  
*Invalid dump frequency*  
Dump frequency must be 1 or greater.  
*Invalid dump image element name*  
The specified element name was not in the standard list of elements. See the dump_modify doc page.
Invalid dump image filename
   The file produced by dump image cannot be binary and must be for a single processor.
Invalid dump image persp value
   Persp value must be >= 0.0.
Invalid dump image theta value
   Theta must be between 0.0 and 180.0 inclusive.
Invalid dump image zoom value
   Zoom value must be > 0.0.
Invalid dump reader style
   Self-explanatory.
Invalid dump style
   The choice of dump style is unknown.
Invalid dump xtc filename
   Filenames used with the dump xtc style cannot be binary or compressed or cause multiple files to be written.
Invalid dump xyz filename
   Filenames used with the dump xyz style cannot be binary or cause files to be written by each processor.
Invalid dump_modify threshold operator
   Operator keyword used for threshold specification in not recognized.
Invalid entry in -reorder file
   Self-explanatory.
Invalid fix ID in variable formula
   The fix is not recognized.
Invalid fix ave/time off column
   Self-explanatory.
Invalid fix box/relax command for a 2d simulation
   Fix box/relax styles involving the z dimension cannot be used in a 2d simulation.
Invalid fix box/relax command pressure settings
   If multiple dimensions are coupled, those dimensions must be specified.
Invalid fix box/relax pressure settings
   Settings for coupled dimensions must be the same.
Invalid fix nvt/npt/nph command for a 2d simulation
   Cannot control z dimension in a 2d model.
Invalid fix nvt/npt/nph command pressure settings
   If multiple dimensions are coupled, those dimensions must be specified.
Invalid fix nvt/npt/nph pressure settings
   Settings for coupled dimensions must be the same.
Invalid fix press/berendsen for a 2d simulation
   The z component of pressure cannot be controlled for a 2d model.
Invalid fix press/berendsen pressure settings
   Settings for coupled dimensions must be the same.
Invalid fix style
   The choice of fix style is unknown.
Invalid flag in force field section of restart file
   Unrecognized entry in restart file.
Invalid flag in header section of restart file
   Unrecognized entry in restart file.
Invalid flag in type arrays section of restart file
   Unrecognized entry in restart file.
Invalid frequency in temper command
   Nevery must be > 0.
Invalid group ID in neigh_modify command
A group ID used in the neigh_modify command does not exist.

*Invalid group function in variable formula*
  Group function is not recognized.

*Invalid group in communicate command*
  Self-explanatory.

*Invalid image color range*
  The lo value in the range is larger than the hi value.

*Invalid image up vector*
  Up vector cannot be (0,0,0).

*Invalid improper style*
  The choice of improper style is unknown.

*Invalid improper type in Impropers section of data file*
  Improper type must be positive integer and within range of specified improper types.

*Invalid keyword in angle table parameters*
  Self-explanatory.

*Invalid keyword in bond table parameters*
  Self-explanatory.

*Invalid keyword in compute angle/local command*
  Self-explanatory.

*Invalid keyword in compute bond/local command*
  Self-explanatory.

*Invalid keyword in compute dihedral/local command*
  Self-explanatory.

*Invalid keyword in compute improper/local command*
  Self-explanatory.

*Invalid keyword in compute pair/local command*
  Self-explanatory.

*Invalid keyword in compute property/atom command*
  Self-explanatory.

*Invalid keyword in compute property/local command*
  Self-explanatory.

*Invalid keyword in compute property/molecule command*
  Self-explanatory.

*Invalid keyword in dump cfg command*
  Self-explanatory.

*Invalid keyword in pair table parameters*
  Keyword used in list of table parameters is not recognized.

*Invalid keyword in thermo_style custom command*
  One or more specified keywords are not recognized.

*Invalid kspace style*
  The choice of kspace style is unknown.

*Invalid length in set command*
  Self-explanatory.

*Invalid mass in set command*
  Self-explanatory.

*Invalid mass line in data file*
  Self-explanatory.

*Invalid mass value*
  Self-explanatory.

*Invalid math function in variable formula*
  Self-explanatory.

*Invalid math/group/special function in variable formula*
Self-explanatory.

Invalid option in lattice command for non-custom style
Certain lattice keywords are not supported unless the lattice style is "custom".

Invalid order of forces within respa levels
For respa, ordering of force computations within respa levels must obey certain rules. E.g. bonds cannot be compute less frequently than angles, pairwise forces cannot be computed less frequently than kspace, etc.

Invalid pair style
The choice of pair style is unknown.

Invalid pair table cutoff
Cutoffs in pair_coeff command are not valid with read-in pair table.

Invalid pair table length
Length of read-in pair table is invalid

Invalid partitions in processors part command
Valid partitions are numbered 1 to N and the sender and receiver cannot be the same partition.

Invalid radius in Atoms section of data file
Radius must be >= 0.0.

Invalid random number seed in fix ttm command
Random number seed must be > 0.

Invalid random number seed in set command
Random number seed must be > 0.

Invalid region style
The choice of region style is unknown.

Invalid replace values in compute reduce
Self-explanatory.

Invalid rigid body ID in fix rigid file
The ID does not match the number or an existing ID of rigid bodies that are defined by the fix rigid command.

Invalid run command N value
The number of timesteps must fit in a 32-bit integer. If you want to run for more steps than this, perform multiple shorter runs.

Invalid run command start/stop value
Self-explanatory.

Invalid run command upto value
Self-explanatory.

Invalid seed for Marsaglia random # generator
The initial seed for this random number generator must be a positive integer less than or equal to 900 million.

Invalid seed for Park random # generator
The initial seed for this random number generator must be a positive integer.

Invalid shape in Ellipsoids section of data file
Self-explanatory.

Invalid shape in Triangles section of data file
Two or more of the triangle corners are duplicate points.

Invalid shape in set command
Self-explanatory.

Invalid shear direction for fix wall/gran
Self-explanatory.

Invalid special function in variable formula
Self-explanatory.

Invalid style in pair_write command
Self-explanatory. Check the input script.
Invalid syntax in variable formula
   Self-explanatory.
Invalid t_event in prd command
   Self-explanatory.
Invalid t_event in tad command
   The value must be greater than 0.
Invalid thermo keyword in variable formula
   The keyword is not recognized.
Invalid tmax in tad command
   The value must be greater than 0.0.
Invalid type for mass set
   Mass command must set a type from 1-N where N is the number of atom types.
Invalid value in set command
   The value specified for the setting is invalid, likely because it is too small or too large.
Invalid variable evaluation in variable formula
   A variable used in a formula could not be evaluated.
Invalid variable in next command
   Self-explanatory.
Invalid variable name
   Variable name used in an input script line is invalid.
Invalid variable name in variable formula
   Variable name is not recognized.
Invalid variable style with next command
   Variable styles equal and world cannot be used in a next command.
Invalid wiggle direction for fix wall/gran
   Self-explanatory.
Invoked angle equil angle on angle style none
   Self-explanatory.
Invoked angle single on angle style none
   Self-explanatory.
Invoked bond equil distance on bond style none
   Self-explanatory.
Invoked bond single on bond style none
   Self-explanatory.
Invoked pair single on pair style none
   A command (e.g. a dump) attempted to invoke the single() function on a pair style none, which is illegal.
   You are probably attempting to compute per-atom quantities with an undefined pair style.
KIM initialization failed
   This is an error generated by the KIM library.
KIM neighbor iterator exceeded range
   This should not happen. It likely indicates a bug in the KIM implementation of the interatomic potential
   where it is requesting neighbors incorrectly.
KIM_DIR environment variable is unset
   This environment variable must be set to use pair_style kim. See the doc page for pair_style kim.
KSpace accuracy too large to estimate G vector
   Paul will doc this.
KSpace style has not yet been set
   Cannot use kspace_modify command until a kspace style is set.
KSpace style is incompatible with Pair style
   Setting a kspace style requires that a pair style with a long-range Coulombic component be selected.
Keyword %s in MEAM parameter file not recognized
   Self-explanatory.
Kspace style does not support compute group/group
Self-explanatory.
Kspace style ppm/tip4p requires newton on
Self-explanatory.
Kspace style requires atom attribute q
The atom style defined does not have these attributes.
Label wasn't found in input script
Self-explanatory.
Lattice orient vectors are not orthogonal
The three specified lattice orientation vectors must be mutually orthogonal.
Lattice orient vectors are not right-handed
The three specified lattice orientation vectors must create a right-handed coordinate system such that a1
cross a2 = a3.
Lattice primitive vectors are collinear
The specified lattice primitive vectors do not form a unit cell with non-zero volume.
Lattice settings are not compatible with 2d simulation
One or more of the specified lattice vectors has a non-zero z component.
Lattice spacings are invalid
Each x,y,z spacing must be > 0.
Lattice style incompatible with simulation dimension
2d simulation can use sq, sq2, or hex lattice. 3d simulation can use sc, bcc, or fcc lattice.
Log of zero/negative value in variable formula
Self-explanatory.
Lost atoms via balance: original %ld current %ld
This should not occur. Report the problem to the developers.
Lost atoms: original %ld current %ld
Lost atoms are checked for each time thermo output is done. See the thermo_modify lost command for
options. Lost atoms usually indicate bad dynamics, e.g. atoms have been blown far out of the simulation
box, or moved further than one processor's sub-domain away before renighboring.
MEAM library error %d
A call to the MEAM Fortran library returned an error.
MPI_LMP_BIGINT and bigint in lmptype.h are not compatible
The size of the MPI datatype does not match the size of a bigint.
MPI_LMP_TAGINT and tagint in lmptype.h are not compatible
The size of the MPI datatype does not match the size of a tagint.
Mass command before simulation box is defined
The mass command cannot be used before a read_data, read_restart, or create_box command.
Min_style command before simulation box is defined
The min_style command cannot be used before a read_data, read_restart, or create_box command.
Minimization could not find thermo_pe compute
This compute is created by the thermo command. It must have been explicitly deleted by a uncompute
command.
Minimize command before simulation box is defined
The minimize command cannot be used before a read_data, read_restart, or create_box command.
Mismatched brackets in variable
Self-explanatory.
Mismatched compute in variable formula
A compute is referenced incorrectly or a compute that produces per-atom values is used in an equal-style
variable formula.
Mismatched fix in variable formula
A fix is referenced incorrectly or a fix that produces per-atom values is used in an equal-style variable
formula.
Mismatched variable in variable formula
A variable is referenced incorrectly or an atom-style variable that produces per-atom values is used in an equal-style variable formula.

Molecular data file has too many atoms
These kinds of data files are currently limited to a number of atoms that fits in a 32-bit integer.

Molecule count changed in compute atom/molecule
Number of molecules must remain constant over time.

Molecule count changed in compute com/molecule
Number of molecules must remain constant over time.

Molecule count changed in compute gyration/molecule
Number of molecules must remain constant over time.

Molecule count changed in compute msd/molecule
Number of molecules must remain constant over time.

Molecule count changed in compute property/molecule
Number of molecules must remain constant over time.

More than one fix deform
Only one fix deform can be defined at a time.

More than one fix freeze
Only one of these fixes can be defined, since the granular pair potentials access it.

More than one fix shake
Only one fix shake can be defined.

Must define angle_style before Angle Coeffs
Must use an angle_style command before reading a data file that defines Angle Coeffs.

Must define angle_style before BondAngle Coeffs
Must use an angle_style command before reading a data file that defines Angle Coeffs.

Must define angle_style before BondBond Coeffs
Must use an angle_style command before reading a data file that defines Angle Coeffs.

Must define bond_style before Bond Coeffs
Must use a bond_style command before reading a data file that defines Bond Coeffs.

Must define dihedral_style before AngleAngleTorsion Coeffs
Must use a dihedral_style command before reading a data file that defines AngleAngleTorsion Coeffs.

Must define dihedral_style before AngleTorsion Coeffs
Must use a dihedral_style command before reading a data file that defines AngleTorsion Coeffs.

Must define dihedral_style before BondBond13 Coeffs
Must use a dihedral_style command before reading a data file that defines BondBond13 Coeffs.

Must define dihedral_style before Dihedral Coeffs
Must use a dihedral_style command before reading a data file that defines Dihedral Coeffs.

Must define dihedral_style before EndBondTorsion Coeffs
Must use a dihedral_style command before reading a data file that defines EndBondTorsion Coeffs.

Must define dihedral_style before MiddleBondTorsion Coeffs
Must use a dihedral_style command before reading a data file that defines MiddleBondTorsion Coeffs.

Must define improper_style before AngleAngle Coeffs
Must use an improper_style command before reading a data file that defines AngleAngle Coeffs.

Must define improper_style before Improper Coeffs
Must use an improper_style command before reading a data file that defines Improper Coeffs.

Must define lattice to append/atoms
A lattice must be defined before using this fix.

Must define pair_style before Pair Coeffs
Must use a pair_style command before reading a data file that defines Pair Coeffs.

Must have more than one processor partition to temper
Cannot use the temper command with only one processor partition. Use the -partition command-line option.
Must read Atoms before Angles
   The Atoms section of a data file must come before an Angles section.
Must read Atoms before Bonds
   The Atoms section of a data file must come before a Bonds section.
Must read Atoms before Dihedrals
   The Atoms section of a data file must come before a Dihedrals section.
Must read Atoms before Ellipsoids
   The Atoms section of a data file must come before a Ellipsoids section.
Must read Atoms before Impropers
   The Atoms section of a data file must come before an Impropers section.
Must read Atoms before Lines
   The Atoms section of a data file must come before a Lines section.
Must read Atoms before Triangles
   The Atoms section of a data file must come before a Triangles section.
Must read Atoms before Velocities
   The Atoms section of a data file must come before a Velocities section.
Must set both respa inner and outer
   Cannot use just the inner or outer option with respa without using the other.
Must shrink-wrap piston boundary
   The boundary style of the face where the piston is applied must be of type s (shrink-wrapped).
Must specify a region in fix deposit
   The region keyword must be specified with this fix.
Must specify a region in fix pour
   The region keyword must be specified with this fix.
Must use -in switch with multiple partitions
   A multi-partition simulation cannot read the input script from stdin. The -in command-line option must be
   used to specify a file.
Must use a block or cylinder region with fix pour
   Self-explanatory.
Must use a block region with fix pour for 2d simulations
   Self-explanatory.
Must use a bond style with TIP4P potential
   TIP4P potentials assume bond lengths in water are constrained by a fix shake command.
Must use a molecular atom style with fix poems molecule
   Self-explanatory.
Must use a z-axis cylinder with fix pour
   The axis of the cylinder region used with the fix pour command must be oriented along the z dimension.
Must use an angle style with TIP4P potential
   TIP4P potentials assume angles in water are constrained by a fix shake command.
Must use atom style with molecule IDs with fix bond/swap
   Self-explanatory.
Must use pair_style comb with fix qeq/comb
   Self-explanatory.
Must use variable energy with fix addforce
   Must define an energy variable when applying a dynamic force during minimization.
NEB command before simulation box is defined
   Self-explanatory.
NEB requires damped dynamics minimizer
   Use a different minimization style.
NEB requires use of fix neb
   Self-explanatory.
NL ramp in wall/piston only implemented in zlo for now
The ramp keyword can only be used for piston applied to face zlo.

**Needed bonus data not in data file**
Some atom styles require bonus data. See the read_data doc page for details.

**Needed topology not in data file**
The header of the data file indicated that bonds or angles or dihedrals or impropers would be included, but they were not present.

**Neigh_modify exclude molecule requires atom attribute molecule**
Self-explanatory.

**Neigh_modify include group != atom_modify.first group**
Self-explanatory.

**Neighbor delay must be 0 or multiple of every setting**
The delay and every parameters set via the neigh_modify command are inconsistent. If the delay setting is non-zero, then it must be a multiple of the every setting.

**Neighbor include group not allowed with ghost neighbors**
This is a current restriction within LAMMPS.

**Neighbor list overflow, boost neigh_modify one**
There are too many neighbors of a single atom. Use the neigh_modify command to increase the max number of neighbors allowed for one atom. You may also want to boost the page size.

**Neighbor list overflow, boost neigh_modify one or page**
There are too many neighbors of a single atom. Use the neigh_modify command to increase the neighbor page size and the max number of neighbors allowed for one atom.

**Neighbor multi not yet enabled for ghost neighbors**
This is a current restriction within LAMMPS.

**Neighbor multi not yet enabled for granular**
Self-explanatory.

**Neighbor multi not yet enabled for rRESPA**
Self-explanatory.

**Neighbor page size must be >= 10x the one atom setting**
This is required to prevent wasting too much memory.

**New bond exceeded bonds per atom in fix bond/create**
See the read_data command for info on setting the "extra bond per atom" header value to allow for additional bonds to be formed.

**New bond exceeded special list size in fix bond/create**
See the special_bonds extra command for info on how to leave space in the special bonds list to allow for additional bonds to be formed.

**Newton bond change after simulation box is defined**
The newton command cannot be used to change the newton bond value after a read_data, read_restart, or create_box command.

**No Kspace style defined for compute group/group**
Self-explanatory.

**No OpenMP support compiled in**
An OpenMP flag is set, but LAMMPS was not built with OpenMP support.

**No angle style is defined for compute angle/local**
Self-explanatory.

**No angles allowed with this atom style**

**No atoms in data file**
The header of the data file indicated that atoms would be included, but they were not present.

**No basis atoms in lattice**
Basis atoms must be defined for lattice style user.

**No bond style is defined for compute bond/local**
Self-explanatory.
No bonds allowed with this atom style

No box information in dump. You have to use 'box no'
Self-explanatory.

No dihedral style is defined for compute dihedral/local
Self-explanatory.

No dihedrals allowed with this atom style

No dump custom arguments specified
The dump custom command requires that atom quantities be specified to output to dump file.

No dump local arguments specified
Self-explanatory.

No ellipsoids allowed with this atom style

No fix gravity defined for fix pour
Cannot add poured particles without gravity to move them.

No improper style is defined for compute improper/local
Self-explanatory.

No impropers allowed with this atom style

No lines allowed with this atom style

No matching element in ADP potential file
The ADP potential file does not contain elements that match the requested elements.

No matching element in EAM potential file
The EAM potential file does not contain elements that match the requested elements.

No overlap of box and region for create_atoms
Self-explanatory.

No pair hbond/dreiding coefficients set
Self-explanatory.

No pair style defined for compute group/group
Cannot calculate group interactions without a pair style defined.

No pair style is defined for compute pair/local
Self-explanatory.

No pair style is defined for compute property/local
Self-explanatory.

No rigid bodies defined
The fix specification did not end up defining any rigid bodies.

No triangles allowed with this atom style

Non digit character between brackets in variable
Self-explanatory.

Non integer # of swaps in temper command
Swap frequency in temper command must evenly divide the total # of timesteps.

Nprocs not a multiple of N for -reorder
Self-explanatory.

Numeric index is out of bounds
A command with an argument that specifies an integer or range of integers is using a value that is less
than 1 or greater than the maximum allowed limit.

One or more atoms belong to multiple rigid bodies
Two or more rigid bodies defined by the fix rigid command cannot contain the same atom.

One or zero atoms in rigid body
Any rigid body defined by the fix rigid command must contain 2 or more atoms.

*Only zhi currently implemented for fix append/atoms*
Self-explanatory.

**Out of range atoms - cannot compute PPPM**
One or more atoms are attempting to map their charge to a PPPM grid point that is not owned by a processor. This is likely for one of two reasons, both of them bad. First, it may mean that an atom near the boundary of a processor's sub-domain has moved more than 1/2 the *neighbor skin distance* without neighbor lists being rebuilt and atoms being migrated to new processors. This also means you may be missing pairwise interactions that need to be computed. The solution is to change the re-neighboring criteria via the `neigh_modify` command. The safest settings are "delay 0 every 1 check yes". Second, it may mean that an atom has moved far outside a processor's sub-domain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

**Overlapping large/large in pair colloid**
This potential is infinite when there is an overlap.

**Overlapping small/large in pair colloid**
This potential is infinite when there is an overlap.

**POEMS fix must come before NPT/NPH fix**
NPT/NPH fix must be defined in input script after all poems fixes, else the fix contribution to the pressure virial is incorrect.

**PPPM grid is too large**
The global PPPM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 4096. You likely need to decrease the requested accuracy.

**PPPM order cannot be < 2 or > than %d**
This is a limitation of the PPPM implementation in LAMMPS.

**PPPM order has been reduced to 0**
LAMMPS has attempted to reduce the PPPM order to enable the simulation to run, but can reduce the order no further. Try increasing the accuracy of PPPM by reducing the tolerance size, thus inducing a larger PPPM grid.

**PRD command before simulation box is defined**
The prd command cannot be used before a read_data, read_restart, or create_box command.

**PRD nsteps must be multiple of t_event**
Self-explanatory.

**PRD t_corr must be multiple of t_event**
Self-explanatory.

**PWD environment variable is unset**
This environment variable must be set to use pair_style kim. See the doc page for pair_style kim.

**Package command after simulation box is defined**
The package command cannot be used after a read_data, read_restart, or create_box command.

**Package cuda command without USER-CUDA installed**
The USER-CUDA package must be installed via "make yes-user-cuda" before LAMMPS is built.

**Pair brownian requires atom style sphere**
Self-explanatory.

**Pair brownian requires extended particles**
One of the particles has radius 0.0.

**Pair brownian requires monodisperse particles**
All particles must be the same finite size.

**Pair brownian/poly requires atom style sphere**
Self-explanatory.

**Pair brownian/poly requires extended particles**
One of the particles has radius 0.0.

**Pair brownian/poly requires newton pair off**
Self-explanatory.
Pair coeff for hybrid has invalid style
   Style in pair coeff must have been listed in pair_style command.

Pair coul/wolf requires atom attribute q
   The atom style defined does not have this attribute.

Pair cutoff < Respa interior cutoff
   One or more pairwise cutoffs are too short to use with the specified rRESPA cutoffs.

Pair dipole/cut requires atom attributes q, mu, torque
   The atom style defined does not have these attributes.

Pair distance < table inner cutoff
   Two atoms are closer together than the pairwise table allows.

Pair distance > table outer cutoff
   Two atoms are further apart than the pairwise table allows.

Pair dpd requires ghost atoms store velocity
   Use the communicate vel yes command to enable this.

Pair gayberne epsilon a,b,c coeffs are not all set
   Each atom type involved in pair_style gayberne must have these 3 coefficients set at least once.

Pair gayberne requires atom style ellipsoid
   Self-explanatory.

Pair gayberne requires atoms with same type have same shape
   Self-explanatory.

Pair gayberne/gpu requires atom style ellipsoid
   Self-explanatory.

Pair gayberne/gpu requires atoms with same type have same shape
   Self-explanatory.

Pair granular requires atom style sphere
   Self-explanatory.

Pair granular requires ghost atoms store velocity
   Use the communicate vel yes command to enable this.

Pair granular with shear history requires newton pair off
   This is a current restriction of the implementation of pair granular styles with history.

Pair hybrid sub-style does not support single call
   You are attempting to invoke a single() call on a pair style that doesn't support it.

Pair hybrid sub-style is not used
   No pair_coeff command used a sub-style specified in the pair_style command.

Pair inner cutoff < Respa interior cutoff
   One or more pairwise cutoffs are too short to use with the specified rRESPA cutoffs.

Pair inner cutoff >= Pair outer cutoff
   The specified cutoffs for the pair style are inconsistent.

Pair line/lj requires atom style line
   Self-explanatory.

Pair lubricate requires atom style sphere
   Self-explanatory.

Pair lubricate requires ghost atoms store velocity
   Use the communicate vel yes command to enable this.

Pair lubricate requires monodisperse particles
   All particles must be the same finite size.

Pair lubricate/poly requires atom style sphere
   Self-explanatory.

Pair lubricate/poly requires extended particles
   One of the particles has radius 0.0.

Pair lubricate/poly requires ghost atoms store velocity
   Use the communicate vel yes command to enable this.
Pair lubricate/poly requires newton pair off
  Self-explanatory.
Pair lubricateU requires atom style sphere
  Self-explanatory.
Pair lubricateU requires ghost atoms store velocity
  Use the communicate vel yes command to enable this.
Pair lubricateU requires monodisperse particles
  All particles must be the same finite size.
Pair lubricateU/poly requires ghost atoms store velocity
  Use the communicate vel yes command to enable this.
Pair lubricateU/poly requires newton pair off
  Self-explanatory.
Pair peri lattice is not identical in x, y, and z
  The lattice defined by the lattice command must be cubic.
Pair peri requires a lattice be defined
  Use the lattice command for this purpose.
Pair peri requires an atom map, see atom_modify
  Even for atomic systems, an atom map is required to find Peridynamic bonds. Use the atom_modify
  command to define one.
Pair resquared epsilon a,b,c coeffs are not all set
  Self-explanatory.
Pair resquared epsilon and sigma coeffs are not all set
  Self-explanatory.
Pair resquared requires atom style ellipsoid
  Self-explanatory.
Pair resquared requires atoms with same type have same shape
  Self-explanatory.
Pair resquared/gpu requires atom style ellipsoid
  Self-explanatory.
Pair resquared/gpu requires atoms with same type have same shape
  Self-explanatory.
Pair style AIREBO requires atom IDs
  This is a requirement to use the AIREBO potential.
Pair style AIREBO requires newton pair on
  See the newton command. This is a restriction to use the AIREBO potential.
Pair style BOP requires atom IDs
  This is a requirement to use the BOP potential.
Pair style BOP requires newton pair on
  See the newton command. This is a restriction to use the BOP potential.
Pair style COMB requires atom IDs
  This is a requirement to use the AIREBO potential.
Pair style COMB requires atom attribute q
  Self-explanatory.
Pair style COMB requires newton pair on
  See the newton command. This is a restriction to use the COMB potential.
Pair style LCBOP requires atom IDs
  This is a requirement to use the LCBOP potential.
Pair style LCBOP requires newton pair on
  See the newton command. This is a restriction to use the LCBOP potential.
Pair style MEAM requires newton pair on
  See the newton command. This is a restriction to use the MEAM potential.
Pair style Stillinger-Weber requires atom IDs
This is a requirement to use the SW potential.

**Pair style Stillinger-Weber requires newton pair on**
See the newton command. This is a restriction to use the SW potential.

**Pair style Tersoff requires atom IDs**
This is a requirement to use the Tersoff potential.

**Pair style Tersoff requires newton pair on**
See the newton command. This is a restriction to use the Tersoff potential.

**Pair style bop requires comm ghost cutoff at least 3x larger than \%g**
Use the communicate ghost command to set this. See the pair bop doc page for more details.

**Pair style born/coul/long requires atom attribute q**
An atom style that defines this attribute must be used.

**Pair style born/coul/wolf requires atom attribute q**
The atom style defined does not have this attribute.

**Pair style buck/coul/cut requires atom attribute q**
The atom style defined does not have this attribute.

**Pair style buck/coul/long requires atom attribute q**
The atom style defined does not have these attributes.

**Pair style buck/coul/long/gpu requires atom attribute q**
The atom style defined does not have this attribute.

**Pair style coul/cut requires atom attribute q**
The atom style defined does not have these attributes.

**Pair style coul/long/gpu requires atom attribute q**
The atom style defined does not have these attributes.

**Pair style does not have extra field requested by compute pair/local**
The pair style does not support the pN value requested by the compute pair/local command.

**Pair style does not support bond_style quartic**
The pair style does not have a single() function, so it cannot be invoked by bond_style quartic.

**Pair style does not support compute group/group**
The pair_style does not have a single() function, so it cannot be invoked by the compute group/group command.

**Pair style does not support compute pair/local**
The pair style does not have a single() function, so it cannot be invoked by compute pair/local.

**Pair style does not support compute property/local**
The pair style does not have a single() function, so it cannot be invoked by fix bond/swap.

**Pair style does not support fix bond/swap**
The pair style does not have a single() function, so it cannot be invoked by fix bond/swap.

**Pair style does not support pair_write**
The pair style does not have a single() function, so it cannot be invoked by pair write.

**Pair style does not support rRESPA inner/middle/outer**
You are attempting to use rRESPA options with a pair style that does not support them.

**Pair style granular with history requires atoms have IDs**
Atoms in the simulation do not have IDs, so history effects cannot be tracked by the granular pair potential.

**Pair style hbond/dreiding requires an atom map, see atom_modify**
Self-explanatory.

**Pair style hbond/dreiding requires atom IDs**
Self-explanatory.

**Pair style hbond/dreiding requires molecular system**
Self-explanatory.

**Pair style hbond/dreiding requires newton pair on**
See the newton command for details.

**Pair style hybrid cannot have hybrid as an argument**
Pair style hybrid cannot have none as an argument
Self-explanatory.

Pair style is incompatible with KSpace style
If a pair style with a long-range Coulombic component is selected, then a kspace style must also be used.

Pair style kim requires newton pair off
This is a current restriction of the KIM library.

Pair style lj/charmm/coul/charmm requires atom attribute q
The atom style defined does not have these attributes.

Pair style lj/charmm/coul/long requires atom attribute q
The atom style defined does not have these attributes.

Pair style lj/charmm/coul/long/gpu requires atom attribute q
The atom style defined does not have this attribute.

Pair style lj/class2/coul/cut requires atom attribute q
The atom style defined does not have this attribute.

Pair style lj/class2/coul/long requires atom attribute q
The atom style defined does not have this attribute.

Pair style lj/class2/coul/long/gpu requires atom attribute q
The atom style defined does not have this attribute.

Pair style lj/cut/coul/cut requires atom attribute q
The atom style defined does not have this attribute.

Pair style lj/cut/coul/cut/gpu requires atom attribute q
The atom style defined does not have this attribute.

Pair style lj/cut/coul/long requires atom attribute q
The atom style defined does not have this attribute.

Pair style lj/cut/coul/long/gpu requires atom attribute q
The atom style defined does not have this attribute.

Pair style lj/cut/coul/long/tip4p requires atom IDs
There are no atom IDs defined in the system and the TIP4P potential requires them to find O,H atoms with a water molecule.

Pair style lj/cut/coul/long/tip4p requires atom attribute q
The atom style defined does not have these attributes.

Pair style lj/cut/coul/long/tip4p requires newton pair on
This is because the computation of constraint forces within a water molecule adds forces to atoms owned by other processors.

Pair style lj/gromacs/coul/gromacs requires atom attribute q
An atom_style with this attribute is needed.

Pair style peri requires atom style peri
Self-explanatory.

Pair style reax requires atom IDs
This is a requirement to use the ReaxFF potential.

Pair style reax requires newton pair on
This is a requirement to use the ReaxFF potential.

Pair table cutoffs must all be equal to use with KSpace
When using pair style table with a long-range KSpace solver, the cutoffs for all atom type pairs must all be the same, since the long-range solver starts at that cutoff.

Pair table parameters did not set N
List of pair table parameters must include N setting.

Pair tersoff/zbl requires metal or real units
This is a current restriction of this pair potential.

Pair tri/lj requires atom style tri
Self-explanatory.
Pair yukawa/colloid requires atom style sphere
  Self-explanatory.
Pair yukawa/colloid requires atoms with same type have same radius
  Self-explanatory.
Pair_coeff command before pair_style is defined
  Self-explanatory.
Pair_coeff command before simulation box is defined
  The pair_coeff command cannot be used before a read_data, read_restart, or create_box command.
Pair_modify command before pair_style is defined
  Self-explanatory.
Pair_write command before pair_style is defined
  Self-explanatory.
Particle on or inside fix wall surface
  Particles must be "exterior" to the wall in order for energy/force to be calculated.
Particle on or inside surface of region used in fix wall/region
  Particles must be "exterior" to the region surface in order for energy/force to be calculated.
Per-atom compute in equal-style variable formula
  Equal-style variables cannot use per-atom quantities.
Per-atom energy was not tallied on needed timestep
  You are using a thermo keyword that requires potentials to have tallied energy, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.
Per-atom fix in equal-style variable formula
  Equal-style variables cannot use per-atom quantities.
Per-atom virial was not tallied on needed timestep
  You are using a thermo keyword that requires potentials to have tallied the virial, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.
Per-processor system is too big
  The number of owned atoms plus ghost atoms on a single processor must fit in 32-bit integer.
Potential energy ID for fix neb does not exist
  Self-explanatory.
Potential energy ID for fix nvt/nph/npt does not exist
  A compute for potential energy must be defined.
Potential file has duplicate entry
  The potential file for a SW or Tersoff potential has more than one entry for the same 3 ordered elements.
Potential file is missing an entry
  The potential file for a SW or Tersoff potential does not have a needed entry.
Power by 0 in variable formula
  Self-explanatory.
Pressure ID for fix box/relax does not exist
  The compute ID needed to compute pressure for the fix does not exist.
Pressure ID for fix modify does not exist
  Self-explanatory.
Pressure ID for fix npt/nph does not exist
  Self-explanatory.
Pressure ID for fix press/berendsen does not exist
  The compute ID needed to compute pressure for the fix does not exist.
Pressure ID for thermo does not exist
  The compute ID needed to compute pressure for thermodynamics does not exist.
Pressure control can not be used with fix nvt
  Self-explanatory.
Pressure control can not be used with fix nvt/asphere
  Self-explanatory.
Pressure control can not be used with fix nvt/sllod  
Self-explanatory.
Pressure control can not be used with fix nvt/sphere  
Self-explanatory.
Pressure control must be used with fix nph  
Self-explanatory.
Pressure control must be used with fix nph/asphere  
Self-explanatory.
Pressure control must be used with fix nph/sphere  
Self-explanatory.
Pressure control must be used with fix nphug  
A pressure control keyword (iso, aniso, tri, x, y, or z) must be provided.
Pressure control must be used with fix npt  
Self-explanatory.
Pressure control must be used with fix npt/asphere  
Self-explanatory.
Pressure control must be used with fix npt/sphere  
Self-explanatory.
Processor count in z must be 1 for 2d simulation  
Self-explanatory.
Processor partitions are inconsistent  
The total number of processors in all partitions must match the number of processors LAMMPS is running on.
Processors command after simulation box is defined  
The processors command cannot be used after a read_data, read_restart, or create_box command.
Processors custom grid file is inconsistent  
The values in the custom file are not consistent with the number of processors you are running on or the Px,Py,Pz settings of the processors command. Or there was not a setting for every processor.
Processors grid numa and map style are incompatible  
Using numa for gstyle in the processors command requires using cart for the map option.
Processors part option and grid style are incompatible  
Cannot use gstyle numa or custom with the part option.
Processors twogrid requires proc count be a multiple of core count  
Self-explanatory.
Pstart and Pstop must have the same value  
Self-explanatory.
R0 < 0 for fix spring command  
Equilibrium spring length is invalid.
Read_dump field not found in dump file  
Self-explanatory.
Read_dump triclinic status does not match simulation  
Both the dump snapshot and the current LAMMPS simulation must be using either an orthogonal or triclinic box.
Read_dump x,y,z fields do not have consistent scaling  
Self-explanatory.
Reax_defs.h setting for NATDEF is too small  
Edit the setting in the ReaxFF library and re-compile the library and re-build LAMMPS.
Reax_defs.h setting for NNEIGHMAXDEF is too small  
Edit the setting in the ReaxFF library and re-compile the library and re-build LAMMPS.
Receiving partition in processors part command is already a receiver  
Cannot specify a partition to be a receiver twice.
Region ID for compute reduce/region does not exist
Region ID for compute temp/region does not exist
Self-explanatory.
Region ID for dump custom does not exist
Self-explanatory.
Region ID for fix addforce does not exist
Self-explanatory.
Region ID for fix ave/spatial does not exist
Self-explanatory.
Region ID for fix aveforce does not exist
Self-explanatory.
Region ID for fix deposit does not exist
Self-explanatory.
Region ID for fix evaporate does not exist
Self-explanatory.
Region ID for fix heat does not exist
Self-explanatory.
Region ID for fix setforce does not exist
Self-explanatory.
Region ID for fix wall/region does not exist
Self-explanatory.
Region ID in variable formula does not exist
Self-explanatory.
Region cannot have 0 length rotation vector
Self-explanatory.
Region intersect region ID does not exist
Self-explanatory.
Region union or intersect cannot be dynamic
The sub-regions can be dynamic, but not the combined region.
Region union region ID does not exist
One or more of the region IDs specified by the region union command does not exist.
Replacing a fix, but new style != old style
A fix ID can be used a 2nd time, but only if the style matches the previous fix. In this case it is assumed
you wish to reset a fix's parameters. This error may mean you are mistakenly re-using a fix ID when you
do not intend to.
Replicate command before simulation box is defined
The replicate command cannot be used before a read_data, read_restart, or create_box command.
Replicate did not assign all atoms correctly
Atoms replicated by the replicate command were not assigned correctly to processors. This is likely due
to some atom coordinates being outside a non-periodic simulation box.
Replicated molecular system atom IDs are too big
See the setting for the allowed atom ID size in the src/lmptype.h file.
Replicated system is too big
See the setting for bigint in the src/lmptype.h file.
Rerun command before simulation box is defined
The rerun command cannot be used before a read_data, read_restart, or create_box command.
Rerun dump file does not contain requested snapshot
Self-explanatory.
Resetting timestep is not allowed with fix move
This is because fix move is moving atoms based on elapsed time.
Respa inner cutoffs are invalid
The first cutoff must be <= the second cutoff.
Respa levels must be $\geq 1$
Self-explanatory.
Respa middle cutoffs are invalid
The first cutoff must be $\leq$ the second cutoff.

Restart variable returned a bad timestep
The variable must return a timestep greater than the current timestep.

Restrain atoms %d %d %d %d missing on proc %d at step %ld
The 4 atoms in a restrain dihedral specified by the fix restrain command are not all accessible to a processor. This probably means an atom has moved too far.

Restrain atoms %d %d %d missing on proc %d at step %ld
The 3 atoms in a restrain angle specified by the fix restrain command are not all accessible to a processor. This probably means an atom has moved too far.

Restrain atoms %d %d missing on proc %d at step %ld
The 2 atoms in a restrain bond specified by the fix restrain command are not all accessible to a processor. This probably means an atom has moved too far.

Reuse of compute ID
A compute ID cannot be used twice.

Reuse of dump ID
A dump ID cannot be used twice.

Reuse of region ID
A region ID cannot be used twice.

Rigid body has degenerate moment of inertia
Fix poems will only work with bodies (collections of atoms) that have non-zero principal moments of inertia. This means they must be 3 or more non-collinear atoms, even with joint atoms removed.

Rigid fix must come before NPT/NPH fix
NPT/NPH fix must be defined in input script after all rigid fixes, else the rigid fix contribution to the pressure virial is incorrect.

Rmask function in equal-style variable formula
Rmask is per-atom operation.

Run command before simulation box is defined
The run command cannot be used before a read_data, read_restart, or create_box command.

Run command start value is after start of run
Self-explanatory.

Run command stop value is before end of run
Self-explanatory.

Run_style command before simulation box is defined
The run_style command cannot be used before a read_data, read_restart, or create_box command.

SRD bin size for fix srd differs from user request
Fix SRD had to adjust the bin size to fit the simulation box. See the cubic keyword if you want this message to be an error vs warning.

SRD bins for fix srd are not cubic enough
The bin shape is not within tolerance of cubic. See the cubic keyword if you want this message to be an error vs warning.

SRD particle %d started inside big particle %d on step %ld bounce %d
See the inside keyword if you want this message to be an error vs warning.

Same dimension twice in fix ave/spatial
Self-explanatory.

Sending partition in processors part command is already a sender
Cannot specify a partition to be a sender twice.

Set command before simulation box is defined
The set command cannot be used before a read_data, read_restart, or create_box command.

Set command with no atoms existing
No atoms are yet defined so the set command cannot be used.

*Set region ID does not exist*
Region ID specified in set command does not exist.

*Shake angles have different bond types*
All 3-atom angle-constrained SHAKE clusters specified by the fix shake command that are the same angle type, must also have the same bond types for the 2 bonds in the angle.

*Shake atoms %d %d %d %d missing on proc %d at step %ld*
The 4 atoms in a single shake cluster specified by the fix shake command are not all accessible to a processor. This probably means an atom has moved too far.

*Shake atoms %d %d %d missing on proc %d at step %ld*
The 3 atoms in a single shake cluster specified by the fix shake command are not all accessible to a processor. This probably means an atom has moved too far.

*Shake atoms %d %d missing on proc %d at step %ld*
The 2 atoms in a single shake cluster specified by the fix shake command are not all accessible to a processor. This probably means an atom has moved too far.

*Shake cluster of more than 4 atoms*
A single cluster specified by the fix shake command can have no more than 4 atoms.

*Shake clusters are connected*
A single cluster specified by the fix shake command must have a single central atom with up to 3 other atoms bonded to it.

*Shake determinant = 0.0*
The determinant of the matrix being solved for a single cluster specified by the fix shake command is numerically invalid.

*Shake fix must come before NPT/NPH fix*
NPT fix must be defined in input script after SHAKE fix, else the SHAKE fix contribution to the pressure virial is incorrect.

*Small, tag, big integers are not sized correctly*
See description of these 3 data types in src/lmptype.h.

*Smallint setting in lmptype.h is invalid*
It has to be the size of an integer.

*Smallint setting in lmptype.h is not compatible*
Smallint stored in restart file is not consistent with LAMMPS version you are running.

*Specified processors != physical processors*
The 3d grid of processors defined by the processors command does not match the number of processors LAMMPS is being run on.

*Specified target stress must be uniaxial or hydrostatic*
Self-explanatory.

*Sqrt of negative value in variable formula*
Self-explanatory.

*Substitution for illegal variable*
Input script line contained a variable that could not be substituted for.

*System in data file is too big*
See the setting for bigint in the src/lmptype.h file.

*TAD nsteps must be multiple of t_event*
Self-explanatory.

*TIP4P hydrogen has incorrect atom type*
The TIP4P pairwise computation found an H atom whose type does not agree with the specified H type.

*TIP4P hydrogen is missing*
The TIP4P pairwise computation failed to find the correct H atom within a water molecule.

*TMD target file did not list all group atoms*
The target file for the fix tmd command did not list all atoms in the fix group.

*Tad command before simulation box is defined*
Tagint setting in lmptype.h is invalid
Tagint must be as large or larger than smallint.

Tagint setting in lmptype.h is not compatible
Smallint stored in restart file is not consistent with LAMMPS version you are running.

Target temperature for fix nvt/npt/nph cannot be 0.0
Self-explanatory.

Target temperature for fix rigid/nvt cannot be 0.0
Self-explanatory.

Temper command before simulation box is defined
The temper command cannot be used before a read_data, read_restart, or create_box command.

Temperature ID for fix bond/swap does not exist
Self-explanatory.

Temperature ID for fix box/relax does not exist
Self-explanatory.

Temperature ID for fix nvt/nph/npt does not exist
Self-explanatory.

Temperature ID for fix press/berendsen does not exist
Self-explanatory.

Temperature ID for fix temp/berendsen does not exist
Self-explanatory.

Temperature ID for fix temp/rescale does not exist
Self-explanatory.

Temperature control can not be used with fix nph
Self-explanatory.

Temperature control can not be used with fix nph/asphere
Self-explanatory.

Temperature control can not be used with fix nph/sphere
Self-explanatory.

Temperature control must be used with fix nphug
The temp keyword must be provided.

Temperature control must be used with fix npt
Self-explanatory.

Temperature control must be used with fix npt/asphere
Self-explanatory.

Temperature control must be used with fix npt/sphere
Self-explanatory.

Temperature control must be used with fix nvt
Self-explanatory.

Temperature control must be used with fix nvt/asphere
Self-explanatory.

Temperature control must be used with fix nvt/sllod
Self-explanatory.

Temperature control must be used with fix nvt/sphere
Self-explanatory.

Temperature for fix nvt/sllod does not have a bias
The specified compute must compute temperature with a bias.

Tempering could not find thermo_pe compute
This compute is created by the thermo command. It must have been explicitly deleted by a uncompute command.

Tempering fix ID is not defined
The fix ID specified by the temper command does not exist.
Tempering temperature fix is not valid
   The fix specified by the temper command is not one that controls temperature (nvt or langevin).

The package gpu command is required for gpu styles
   Self-explanatory.

Thermo and fix not computed at compatible times
   Fixes generate values on specific timesteps. The thermo output does not match these timesteps.

Thermo compute array is accessed out-of-range
   Self-explanatory.

Thermo compute does not compute array
   Self-explanatory.

Thermo compute does not compute scalar
   Self-explanatory.

Thermo compute does not compute vector
   Self-explanatory.

Thermo compute vector is accessed out-of-range
   Self-explanatory.

Thermo custom variable cannot be indexed
   Self-explanatory.

Thermo custom variable is not equal-style variable
   Only equal-style variables can be output with thermodynamics, not atom-style variables.

Thermo every variable returned a bad timestep
   The variable must return a timestep greater than the current timestep.

Thermo fix array is accessed out-of-range
   Self-explanatory.

Thermo fix does not compute array
   Self-explanatory.

Thermo fix does not compute scalar
   Self-explanatory.

Thermo fix does not compute vector
   Self-explanatory.

Thermo fix vector is accessed out-of-range
   Self-explanatory.

Thermo keyword in variable requires lattice be defined
   The xlat, ylat, zlat keywords refer to lattice properties.

Thermo keyword in variable requires thermo to use/init pe
   You are using a thermo keyword in a variable that requires potential energy to be calculated, but your
   thermo output does not use it. Add it to your thermo output.

Thermo keyword in variable requires thermo to use/init press
   You are using a thermo keyword in a variable that requires pressure to be calculated, but your thermo
   output does not use it. Add it to your thermo output.

Thermo keyword in variable requires thermo to use/init temp
   You are using a thermo keyword in a variable that requires temperature to be calculated, but your thermo
   output does not use it. Add it to your thermo output.

Thermo keyword requires lattice be defined
   The xlat, ylat, zlat keywords refer to lattice properties.

Thermo style does not use press
   Cannot use thermo_modify to set this parameter since the thermo_style is not computing this quantity.

Thermo style does not use temp
   Cannot use thermo_modify to set this parameter since the thermo_style is not computing this quantity.

Thermo_modify int format does not contain d character
   Self-explanatory.

Thermo_modify pressure ID does not compute pressure
The specified compute ID does not compute pressure.

Thermo_modify temperature ID does not compute temperature

The specified compute ID does not compute temperature.

Thermo_style command before simulation box is defined

The thermo_style command cannot be used before a read_data, read_restart, or create_box command.

This variable thermo keyword cannot be used between runs

Keywords that refer to time (such as cpu, elapsed) do not make sense in between runs.

Threshold for an atom property that isn't allocated

A dump threshold has been requested on a quantity that is not defined by the atom style used in this simulation.

Timestep must be >= 0

Specified timestep is invalid.

Too big a problem to use velocity create loop all

The system size must fit in a 32-bit integer to use this option.

Too big a timestep

Specified timestep is too large.

Too big a timestep for dump dcd

The timestep must fit in a 32-bit integer to use this dump style.

Too big a timestep for dump xtc

The timestep must fit in a 32-bit integer to use this dump style.

Too few bits for lookup table

Table size specified via pair_modify command does not work with your machine's floating point representation.

Too many atom pairs for pair bop

The number of atomic pairs exceeds the expected number. Check your atomic structure to ensure that it is realistic.

Too many atom sorting bins

This is likely due to an immense simulation box that has blown up to a large size.

Too many atom triplets for pair bop

The number of three atom groups for angle determinations exceeds the expected number. Check your atomic structure to ensure that it is realistic.

Too many atoms for dump dcd

The system size must fit in a 32-bit integer to use this dump style.

Too many atoms for dump xtc

The system size must fit in a 32-bit integer to use this dump style.

Too many atoms to dump sort

Cannot sort when running with more than 2^31 atoms.

Too many exponent bits for lookup table

Table size specified via pair_modify command does not work with your machine's floating point representation.

Too many groups

The maximum number of atom groups (including the "all" group) is given by MAX_GROUP in group.cpp and is 32.

Too many iterations

You must use a number of iterations that fit in a 32-bit integer for minimization.

Too many local+ghost atoms for neighbor list

The number of nlocal + nghost atoms on a processor is limited by the size of a 32-bit integer with 2 bits removed for masking 1-2, 1-3, 1-4 neighbors.

Too many mantissa bits for lookup table

Table size specified via pair_modify command does not work with your machine's floating point representation.

Too many masses for fix shake
The fix shake command cannot list more masses than there are atom types.

Too many neighbor bins
This is likely due to an immense simulation box that has blown up to a large size.

Too many timesteps
The cumulative timesteps must fit in a 64-bit integer.

Too many timesteps for NEB
You must use a number of timesteps that fit in a 32-bit integer for NEB.

Too many total atoms
See the setting for bigint in the src/lmptype.h file.

Too many total bits for bitmapped lookup table
Table size specified via pair_modify command is too large. Note that a value of N generates a 2^N size table.

Too many touching neighbors - boost MAXTOUCH
A granular simulation has too many neighbors touching one atom. The MAXTOUCH parameter in fix_shear_history.cpp must be set larger and LAMMPS must be re-built.

Too much per-proc info for dump
Number of local atoms times number of columns must fit in a 32-bit integer for dump.

Tree structure in joint connections
Fix poems cannot (yet) work with coupled bodies whose joints connect the bodies in a tree structure.

Triclinic box skew is too large
The displacement in a skewed direction must be less than half the box length in that dimension. E.g. the xy tilt must be between -half and +half of the x box length.

Tried to convert a double to int, but input_double > INT_MAX
Self-explanatory.

Two groups cannot be the same in fix spring couple
Self-explanatory.

USER-CUDA mode requires CUDA variant of min style
CUDA mode is enabled, so the min style must include a cuda suffix.

USER-CUDA mode requires CUDA variant of run style
CUDA mode is enabled, so the run style must include a cuda suffix.

USER-CUDA package requires a cuda enabled atom_style
Self-explanatory.

Unable to initialize accelerator for use
There was a problem initializing an accelerator for the gpu package.

Unbalanced quotes in input line
No matching end double quote was found following a leading double quote.

Unexpected end of -reorder file
Self-explanatory.

Unexpected end of custom file
Self-explanatory.

Unexpected end of data file
LAMMPS hit the end of the data file while attempting to read a section. Something is wrong with the format of the data file.

Unexpected end of dump file
A read operation from the file failed.

Unexpected end of fix rigid file
A read operation from the file failed.

Units command after simulation box is defined
The units command cannot be used after a read_data, read_restart, or create_box command.

Universe/uloop variable count < # of partitions
A universe or uloop style variable must specify a number of values >= to the number of processor partitions.
Unknown command: %s
The command is not known to LAMMPS. Check the input script.

Unknown error in GPU library
Self-explanatory.

Unknown identifier in data file: %s
A section of the data file cannot be read by LAMMPS.

Unknown table style in angle style table
Self-explanatory.

Unknown table style in bond style table
Self-explanatory.

Unknown table style in pair_style command
Style of table is invalid for use with pair_style table command.

Unrecognized lattice type in MEAM file 1
The lattice type in an entry of the MEAM library file is not valid.

Unrecognized lattice type in MEAM file 2
The lattice type in an entry of the MEAM parameter file is not valid.

Unrecognized pair style in compute pair command
Self-explanatory.

Use of change_box with undefined lattice
Must use lattice command with change_box command if units option is set to lattice.

Use of compute temp/ramp with undefined lattice
Must use lattice command with compute temp/ramp command if units option is set to lattice.

Use of displace_atoms with undefined lattice
Must use lattice command with displace_atoms command if units option is set to lattice.

Use of fix append/atoms with undefined lattice
A lattice must be defined before using this fix.

Use of fix ave/spatial with undefined lattice
A lattice must be defined to use fix ave/spatial with units = lattice.

Use of fix deform with undefined lattice
A lattice must be defined to use fix deform with units = lattice.

Use of fix deposit with undefined lattice
Must use lattice command with compute fix deposit command if units option is set to lattice.

Use of fix dt/reset with undefined lattice
Must use lattice command with fix dt/reset command if units option is set to lattice.

Use of fix indent with undefined lattice
The lattice command must be used to define a lattice before using the fix indent command.

Use of fix move with undefined lattice
Must use lattice command with fix move command if units option is set to lattice.

Use of fix recenter with undefined lattice
Must use lattice command with fix recenter command if units option is set to lattice.

Use of fix wall with undefined lattice
Must use lattice command with fix wall command if units option is set to lattice.

Use of fix wall/piston with undefined lattice
A lattice must be defined before using this fix.

Use of region with undefined lattice
If units = lattice (the default) for the region command, then a lattice must first be defined via the lattice command.

Use of velocity with undefined lattice
If units = lattice (the default) for the velocity set or velocity ramp command, then a lattice must first be defined via the lattice command.

Using fix nvt/sllod with inconsistent fix deform remap option
Fix nvt/sllod requires that deforming atoms have a velocity profile provided by "remap v" as a fix deform
option.

Using fix nvt/sllod with no fix deform defined
Self-explanatory.

Using fix srd with inconsistent fix deform remap option
When shearing the box in an SRD simulation, the remap v option for fix deform needs to be used.

Using pair lubricate with inconsistent fix deform remap option
Must use remap v option with fix deform with this pair style.

Using pair lubricate/poly with inconsistent fix deform remap option
If fix deform is used, the remap v option is required.

Variable evaluation before simulation box is defined
Cannot evaluate a compute or fix or atom-based value in a variable before the simulation has been setup.

Variable for compute ti is invalid style
Self-explanatory.

Variable for dump every is invalid style
Only equal-style variables can be used.

Variable for dump image center is invalid style
Must be an equal-style variable.

Variable for dump image persp is invalid style
Must be an equal-style variable.

Variable for dump image phi is invalid style
Must be an equal-style variable.

Variable for dump image theta is invalid style
Must be an equal-style variable.

Variable for dump image zoom is invalid style
Must be an equal-style variable.

Variable for fix adapt is invalid style
Only equal-style variables can be used.

Variable for fix addforce is invalid style
Self-explanatory.

Variable for fix aveforce is invalid style
Only equal-style variables can be used.

Variable for fix deform is invalid style
The variable must be an equal-style variable.

Variable for fix efield is invalid style
Only equal-style variables can be used.

Variable for fix gravity is invalid style
Only equal-style variables can be used.

Variable for fix indent is invalid style
Only equal-style variables can be used.

Variable for fix indent is not equal style
Only equal-style variables can be used.

Variable for fix langevin is invalid style
It must be an equal-style variable.

Variable for fix move is invalid style
Only equal-style variables can be used.

Variable for fix setforce is invalid style
Only equal-style variables can be used.

Variable for fix temp/berendsen is invalid style
Only equal-style variables can be used.

Variable for fix temp/rescale is invalid style
Only equal-style variables can be used.

Variable for fix wall is invalid style
Only equal-style variables can be used.

Variable for fix wall/reflect is invalid style
Only equal-style variables can be used.

Variable for fix wall/srd is invalid style
Only equal-style variables can be used.

Variable for region is invalid style
Only equal-style variables can be used.

Variable for region is not equal style
Self-explanatory.

Variable for restart is invalid style
Only equal-style variables can be used.

Variable for thermo every is invalid style
Only equal-style variables can be used.

Variable for velocity set is invalid style
Only atom-style variables can be used.

Variable formula compute array is accessed out-of-range
Self-explanatory.

Variable formula compute vector is accessed out-of-range
Self-explanatory.

Variable formula fix array is accessed out-of-range
Self-explanatory.

Variable formula fix vector is accessed out-of-range
Self-explanatory.

Variable name for compute atom/molecule does not exist
Self-explanatory.

Variable name for compute reduce does not exist
Self-explanatory.

Variable name for compute ti does not exist
Self-explanatory.

Variable name for dump every does not exist
Self-explanatory.

Variable name for dump image center does not exist
Self-explanatory.

Variable name for dump image persp does not exist
Self-explanatory.

Variable name for dump image phi does not exist
Self-explanatory.

Variable name for dump image theta does not exist
Self-explanatory.

Variable name for dump image zoom does not exist
Self-explanatory.

Variable name for fix adapt does not exist
Self-explanatory.

Variable name for fix addforce does not exist
Self-explanatory.

Variable name for fix ave/atom does not exist
Self-explanatory.

Variable name for fix ave/correlate does not exist
Self-explanatory.

Variable name for fix ave/histo does not exist
Self-explanatory.

Variable name for fix ave/spatial does not exist
Variable name for fix ave/time does not exist
Self-explanatory.
Variable name for fix aveforce does not exist
Self-explanatory.
Variable name for fix deform does not exist
Self-explanatory.
Variable name for fix efield does not exist
Self-explanatory.
Variable name for fix gravity does not exist
Self-explanatory.
Variable name for fix indent does not exist
Self-explanatory.
Variable name for fix langevin does not exist
Self-explanatory.
Variable name for fix move does not exist
Self-explanatory.
Variable name for fix setforce does not exist
Self-explanatory.
Variable name for fix store/state does not exist
Self-explanatory.
Variable name for fix temp/berendsen does not exist
Self-explanatory.
Variable name for fix temp/rescale does not exist
Self-explanatory.
Variable name for fix wall does not exist
Self-explanatory.
Variable name for fix wall/reflect does not exist
Self-explanatory.
Variable name for fix wall/srd does not exist
Self-explanatory.
Variable name for region does not exist
Self-explanatory.
Variable name for restart does not exist
Self-explanatory.
Variable name for thermo every does not exist
Self-explanatory.
Variable name for velocity set does not exist
Self-explanatory.
Variable name must be alphanumeric or underscore characters
Self-explanatory.
Velocity command before simulation box is defined
The velocity command cannot be used before a read_data, read_restart, or create_box command.
Velocity command with no atoms existing
A velocity command has been used, but no atoms yet exist.
Velocity ramp in z for a 2d problem
Self-explanatory.
Velocity temperature ID does not compute temperature
The compute ID given to the velocity command must compute temperature.
Verlet/split requires 2 partitions
See the -partition command-line switch.
Verlet/split requires Rspace partition layout be multiple of Kspace partition layout in each dim
This is controlled by the processors command.

Verlet/split requires Rspace partition size be multiple of Kspace partition size
This is so there is an equal number of Rspace processors for every Kspace processor.

Virial was not tallied on needed timestep
You are using a thermo keyword that requires potentials to have tallied the virial, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

Wall defined twice in fix wall command
Self-explanatory.

Wall defined twice in fix wall/reflect command
Self-explanatory.

Wall defined twice in fix wall/srd command
Self-explanatory.

Water H epsilon must be 0.0 for pair style lj/cut/coul/long/tip4p
This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

World variable count doesn't match # of partitions
A world-style variable must specify a number of values equal to the number of processor partitions.

Write_restart command before simulation box is defined
The write_restart command cannot be used before a read_data, read_restart, or create_box command.

Zero-length lattice orient vector
Self-explanatory.

Warnings:

Atom with molecule ID = 0 included in compute molecule group
The group used in a compute command that operates on molecules includes atoms with no molecule ID. This is probably not what you want.

Both groups in compute group/group have a net charge; the Kspace boundary correction to energy will be non-zero
Self-explanatory.

Broken bonds will not alter angles, dihedrals, or impropers
See the doc page for fix bond/break for more info on this restriction.

Building an occasional neighbor list when atoms may have moved too far
This can cause LAMMPS to crash when the neighbor list is built. The solution is to check for building the regular neighbor lists more frequently.

Cannot include log terms without 1/r terms; setting flagHI to 1
Self-explanatory.

Cannot include log terms without 1/r terms; setting flagHI to 1.
Self-explanatory.

Compute cna/atom cutoff may be too large to find ghost atom neighbors
The neighbor cutoff used may not encompass enough ghost atoms to perform this operation correctly.

Computing temperature of portions of rigid bodies
The group defined by the temperature compute does not encompass all the atoms in one or more rigid bodies, so the change in degrees-of-freedom for the atoms in those partial rigid bodies will not be accounted for.

Created bonds will not create angles, dihedrals, or impropers
See the doc page for fix bond/create for more info on this restriction.

Dihedral problem: %d %ld %d %d %d %d
Conformation of the 4 listed dihedral atoms is extreme; you may want to check your simulation geometry.

Dump dcd/xtc timestamp may be wrong with fix dt/reset
If the fix changes the timestep, the dump dcd file will not reflect the change.

FENE bond too long: %ld %d %d %g
A FENE bond has stretched dangerously far. It's interaction strength will be truncated to attempt to prevent the bond from blowing up.

FENE bond too long: %ld %g
A FENE bond has stretched dangerously far. It's interaction strength will be truncated to attempt to prevent the bond from blowing up.

Fix GCMC may delete atom with non-zero molecule ID
This is probably an error, since you should not delete only one atom of a molecule. The GCMC molecule exchange feature does not yet work.

Fix SRD walls overlap but fix srd overlap not set
You likely want to set this in your input script.

Fix bond/swap will ignore defined angles
See the doc page for fix bond/swap for more info on this restriction.

Fix evaporate may delete atom with non-zero molecule ID
This is probably an error, since you should not delete only one atom of a molecule.

Fix move does not update angular momentum
Atoms store this quantity, but fix move does not (yet) update it.

Fix move does not update quaternions
Atoms store this quantity, but fix move does not (yet) update it.

Fix recenter should come after all other integration fixes
Other fixes may change the position of the center-of-mass, so fix recenter should come last.

Fix shake with rRESPA computes invalid pressures
This is a known bug in LAMMPS that has not yet been fixed. If you use SHAKE with rRESPA and perform a constant volume simulation (e.g. using fix npt) this only affects the output pressure, not the dynamics of the simulation. If you use SHAKE with rRESPA and perform a constant pressure simulation (e.g. using fix npt) then you will be equilibrating to the wrong volume.

Fix srdf SRD moves may trigger frequent reneighboring
This is because the SRD particles may move long distances.

Fix srdf grid size > 1/4 of big particle diameter
This may cause accuracy problems.

Fix srdf particle moved outside valid domain
This may indicate a problem with your simulation parameters.

Fix srdf particles may move > big particle diameter
This may cause accuracy problems.

Fix srdf viscosity < 0.0 due to low SRD density
This may cause accuracy problems.

Fix thermal/conductivity comes before fix ave/spatial
The order of these 2 fixes in your input script is such that fix thermal/conductivity comes first. If you are using fix ave/spatial to measure the temperature profile induced by fix viscosity, then this may cause a glitch in the profile since you are averaging immediately after swaps have occurred. Flipping the order of the 2 fixes typically helps.

Fix viscosity comes before fix ave/spatial
The order of these 2 fixes in your input script is such that fix viscosity comes first. If you are using fix ave/spatial to measure the velocity profile induced by fix viscosity, then this may cause a glitch in the profile since you are averaging immediately after swaps have occurred. Flipping the order of the 2 fixes typically helps.

Group for fix modify temp != fix group
The fix_modify command is specifying a temperature computation that computes a temperature on a different group of atoms than the fix itself operates on. This is probably not what you want to do.

Improper problem: %d %ld %d %d %d %d
Conformation of the 4 listed improper atoms is extreme; you may want to check your simulation geometry.

Kspace_modify slab param < 2.0 may cause unphysical behavior
The kspace_modify slab parameter should be larger to insure periodic grids padded with empty space do not overlap.

Less insertions than requested
Less atom insertions occurred on this timestep due to the fix pour command than were scheduled. This is probably because there were too many overlaps detected.

Lost atoms via change_box: original %ld current %ld
The command options you have used caused atoms to be lost.

Lost atoms via displace_atoms: original %ld current %ld
The command options you have used caused atoms to be lost.

Lost atoms: original %ld current %ld
Lost atoms are checked for each time thermo output is done. See the thermo_modify lost command for options. Lost atoms usually indicate bad dynamics, e.g. atoms have been blown far out of the simulation box, or moved further than one processor's sub-domain away before reneighboring.

Mismatch between velocity and compute groups
The temperature computation used by the velocity command will not be on the same group of atoms that velocities are being set for.

More than one compute centro/atom
It is not efficient to use compute centro/atom more than once.

More than one compute cluster/atom
It is not efficient to use compute cluster/atom more than once.

More than one compute cna/atom defined
It is not efficient to use compute cna/atom more than once.

More than one compute coord/atom
It is not efficient to use compute coord/atom more than once.

More than one compute damage/atom
It is not efficient to use compute ke/atom more than once.

More than one compute ke/atom
It is not efficient to use compute ke/atom more than once.

More than one fix poems
It is not efficient to use fix poems more than once.

More than one fix rigid
It is not efficient to use fix rigid more than once.

New thermo_style command, previous thermo_modify settings will be lost
If a thermo_style command is used after a thermo_modify command, the settings changed by the thermo_modify command will be reset to their default values. This is because the thermo_modify command acts on the currently defined thermo style, and a thermo_style command creates a new style.

No Kspace calculation with verlet/split
The 2nd partition performs a kspace calculation so the kspace_style command must be used.

No fixes defined, atoms won't move
If you are not using a fix like nve, nvt, npt then atom velocities and coordinates will not be updated during timestepping.

No joints between rigid bodies, use fix rigid instead
The bodies defined by fix poems are not connected by joints. POEMS will integrate the body motion, but it would be more efficient to use fix rigid.

Not using real units with pair reax
This is most likely an error, unless you have created your own ReaxFF parameter file in a different set of units.

One or more atoms are time integrated more than once
This is probably an error since you typically do not want to advance the positions or velocities of an atom more than once per timestep.

One or more compute molecules has atoms not in group
The group used in a compute command that operates on molecules does not include all the atoms in some
molecules. This is probably not what you want.

One or more respa levels compute no forces
This is computationally inefficient.

Pair COMB charge %.10f with force %.10f hit max barrier
Something is possibly wrong with your model.
Pair COMB charge %.10f with force %.10f hit min barrier
Something is possibly wrong with your model.
Pair brownian needs newton pair on for momentum conservation
Self-explanatory.
Pair dpd needs newton pair on for momentum conservation
Self-explanatory.
Pair dsmc: num_of_collisions > number_of_A
Collision model in DSMC is breaking down.
Pair dsmc: num_of_collisions > number_of_B
Collision model in DSMC is breaking down.

Particle deposition was unsuccessful
The fix deposit command was not able to insert as many atoms as needed. The requested volume fraction may be too high, or other atoms may be in the insertion region.

Reducing PPPM order b/c stencil extends beyond neighbor processor
LAMMPS is attempting this in order to allow the simulation to run. It should not effect the PPPM accuracy.

Replacing a fix, but new group != old group
The ID and style of a fix match for a fix you are changing with a fix command, but the new group you are specifying does not match the old group.

Replicating in a non-periodic dimension
The parameters for a replicate command will cause a non-periodic dimension to be replicated; this may cause unwanted behavior.

Resetting reneighboring criteria during PRD
A PRD simulation requires that neigh_modify settings be delay = 0, every = 1, check = yes. Since these settings were not in place, LAMMPS changed them and will restore them to their original values after the PRD simulation.

Resetting reneighboring criteria during TAD
A TAD simulation requires that neigh_modify settings be delay = 0, every = 1, check = yes. Since these settings were not in place, LAMMPS changed them and will restore them to their original values after the PRD simulation.

Resetting reneighboring criteria during minimization
Minimization requires that neigh_modify settings be delay = 0, every = 1, check = yes. Since these settings were not in place, LAMMPS changed them and will restore them to their original values after the minimization.

Restart file used different # of processors
The restart file was written out by a LAMMPS simulation running on a different number of processors. Due to round-off, the trajectories of your restarted simulation may diverge a little more quickly than if you ran on the same # of processors.

Restart file used different 3d processor grid
The restart file was written out by a LAMMPS simulation running on a different 3d grid of processors. Due to round-off, the trajectories of your restarted simulation may diverge a little more quickly than if you ran on the same # of processors.

Restart file used different boundary settings, using restart file values
Your input script cannot change these restart file settings.

Restart file used different newton bond setting, using restart file value
The restart file value will override the setting in the input script.

Restart file used different newton pair setting, using input script value
The input script value will override the setting in the restart file.

**Restart file version does not match LAMMPS version**
This may cause problems when reading the restart file.

**Restrain problem: %d %ld %d %d %d %d**
Conformation of the 4 listed dihedral atoms is extreme; you may want to check your simulation geometry.

**Running PRD with only one replica**
This is allowed, but you will get no parallel speed-up.

**SRD bin shifting turned on due to small lambda**
This is done to try to preserve accuracy.

**SRD bin size for fix srd differs from user request**
Fix SRD had to adjust the bin size to fit the simulation box. See the cubic keyword if you want this message to be an error vs warning.

**SRD bins for fix srd are not cubic enough**
The bin shape is not within tolerance of cubic. See the cubic keyword if you want this message to be an error vs warning.

**SRD particle %d started inside big particle %d on step %ld bounce %d**
See the inside keyword if you want this message to be an error vs warning.

**Shake determinant < 0.0**
The determinant of the quadratic equation being solved for a single cluster specified by the fix shake command is numerically suspect. LAMMPS will set it to 0.0 and continue.

**Should not allow rigid bodies to bounce off reflecting walls**
LAMMPS allows this, but their dynamics are not computed correctly.

**System is not charge neutral, net charge = %g**
The total charge on all atoms on the system is not 0.0, which is not valid for Ewald or PPPM.

**Table inner cutoff >= outer cutoff**
You specified an inner cutoff for a Coulombic table that is longer than the global cutoff. Probably not what you wanted.

**Temperature for MSST is not for group all**
User-assigned temperature to MSST fix does not compute temperature for all atoms. Since MSST computes a global pressure, the kinetic energy contribution from the temperature is assumed to also be for all atoms. Thus the pressure used by MSST could be inaccurate.

**Temperature for NPT is not for group all**
User-assigned temperature to NPT fix does not compute temperature for all atoms. Since NPT computes a global pressure, the kinetic energy contribution from the temperature is assumed to also be for all atoms. Thus the pressure used by NPT could be inaccurate.

**Temperature for fix modify is not for group all**
The temperature compute is being used with a pressure calculation which does operate on group all, so this may be inconsistent.

**Temperature for thermo pressure is not for group all**
User-assigned temperature to thermo via the thermo_modify command does not compute temperature for all atoms. Since thermo computes a global pressure, the kinetic energy contribution from the temperature is assumed to also be for all atoms. Thus the pressure printed by thermo could be inaccurate.

**Too many common neighbors in CNA %d times**
More than the maximum # of neighbors was found multiple times. This was unexpected.

**Too many inner timesteps in fix ttm**
Self-explanatory.

**Too many neighbors in CNA for %d atoms**
More than the maximum # of neighbors was found multiple times. This was unexpected.

**Use special bonds = 0,1,1 with bond style fene**
Most FENE models need this setting for the special_bonds command.

**Use special bonds = 0,1,1 with bond style fene/expand**
Most FENE models need this setting for the special_bonds command.
Using *compute temp/deform with inconsistent fix deform remap option*

Fix nvt/sllod assumes deforming atoms have a velocity profile provided by "remap v" or "remap none" as a fix deform option.

**Using compute temp/deform with no fix deform defined**

This is probably an error, since it makes little sense to use compute temp/deform in this case.

**Using fix srd with box deformation but no SRD thermostat**

The deformation will heat the SRD particles so this can be dangerous.

**Using pair tail corrections with nonperiodic system**

This is probably a bogus thing to do, since tail corrections are computed by integrating the density of a periodic system out to infinity.
13. Future and history

This section lists features we plan to add to LAMMPS, features of previous versions of LAMMPS, and features of other parallel molecular dynamics codes our group has distributed.

13.1 Coming attractions

The Wish list link on the LAMMPS WWW page gives a list of features we are hoping to add to LAMMPS in the future, including contact names of individuals you can email if you are interested in contributing to the development or would be a future user of that feature.

You can also send email to the developers if you want to add your wish to the list.

13.2 Past versions

LAMMPS development began in the mid 1990s under a cooperative research & development agreement (CRADA) between two DOE labs (Sandia and LLNL) and 3 companies (Cray, Bristol Myers Squibb, and Dupont). The goal was to develop a large-scale parallel classical MD code; the coding effort was led by Steve Plimpton at Sandia.

After the CRADA ended, a final F77 version, LAMMPS 99, was released. As development of LAMMPS continued at Sandia, its memory management was converted to F90; a final F90 version was released as LAMMPS 2001.

The current LAMMPS is a rewrite in C++ and was first publicly released as an open source code in 2004. It includes many new features beyond those in LAMMPS 99 or 2001. It also includes features from older parallel MD codes written at Sandia, namely ParaDyn, Warp, and GranFlow (see below).

In late 2006 we began merging new capabilities into LAMMPS that were developed by Aidan Thompson at Sandia for his MD code GRASP, which has a parallel framework similar to LAMMPS. Most notably, these have included many-body potentials - Stillinger-Weber, Tersoff, ReaxFF - and the associated charge-equilibration routines needed for ReaxFF.

The History link on the LAMMPS WWW page gives a timeline of features added to the C++ open-source version of LAMMPS over the last several years.

These older codes are available for download from the LAMMPS WWW site, except for Warp & GranFlow which were primarily used internally. A brief listing of their features is given here.

LAMMPS 2001

- F90 + MPI
- dynamic memory
- spatial-decomposition parallelism
- NVE, NVT, NPT, NPH, rRESPA integrators
- LJ and Coulombic pairwise force fields
- all-atom, united-atom, bead-spring polymer force fields
- CHARMM-compatible force fields
- class 2 force fields
- 3d/2d Ewald & PPPM
- various force and temperature constraints
- SHAKE
- Hessian-free truncated-Newton minimizer
- user-defined diagnostics

LAMMPS 99

- F77 + MPI
- static memory allocation
- spatial-decomposition parallelism
- most of the LAMMPS 2001 features with a few exceptions
- no 2d Ewald & PPPM
- molecular force fields are missing a few CHARMM terms
- no SHAKE

Warp

- F90 + MPI
- spatial-decomposition parallelism
- embedded atom method (EAM) metal potentials + LJ
- lattice and grain-boundary atom creation
- NVE, NVT integrators
- boundary conditions for applying shear stresses
- temperature controls for actively sheared systems
- per-atom energy and centro-symmetry computation and output

ParaDyn

- F77 + MPI
- atom- and force-decomposition parallelism
- embedded atom method (EAM) metal potentials
- lattice atom creation
- NVE, NVT, NPT integrators
- all serial DYNAMO features for controls and constraints

GranFlow

- F90 + MPI
- spatial-decomposition parallelism
- frictional granular potentials
- NVE integrator
- boundary conditions for granular flow and packing and walls
- particle insertion
angle_style charmm command

angle_style charmm/omp command

Syntax:

angle_style charmm

Examples:

angle_style charmm
angle_coeff 1 300.0 107.0 50.0 3.0

Description:

The charmm angle style uses the potential

\[ E = K(\theta - \theta_0)^2 + K_{UB}(r - r_{UB})^2 \]

with an additional Urey_Bradley term based on the distance \( r \) between the 1st and 3rd atoms in the angle. \( K, \theta_0, K_{ub}, \) and \( r_{ub} \) are coefficients defined for each angle type.

See (MacKerell) for a description of the CHARMM force field.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- \( K \) (energy/radian^2)
- \( \theta_0 \) (degrees)
- \( K_{ub} \) (energy/distance^2)
- \( r_{ub} \) (distance)

\( \theta_0 \) is specified in degrees, but LAMMPS converts it to radians internally; hence the units of \( K \) are in energy/radian^2.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.
See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**

This angle style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

**Related commands:**

angle_coeff

**Default:** none

angle_style class2 command

angle_style class2/omp command

Syntax:

angle_style class2

Examples:

angle_style class2
angle_coeff * 75.0
angle_coeff 1 bb 10.5872 1.0119 1.5228
angle_coeff * ba 3.6551 24.895 1.0119 1.5228

Description:

The class2 angle style uses the potential

\[ E = E_a + E_{bb} + E_{ba} \]

\[ E_a = K_2(\theta - \theta_0)^2 + K_3(\theta - \theta_0)^3 + K_4(\theta - \theta_0)^4 \]

\[ E_{bb} = M(r_{ij} - r_1)(r_{jk} - r_2) \]

\[ E_{ba} = N_1(r_{ij} - r_1)(\theta - \theta_0) + N_2(r_{jk} - r_2)(\theta - \theta_0) \]

where \( E_a \) is the angle term, \( E_{bb} \) is a bond-bond term, and \( E_{ba} \) is a bond-angle term. \( \theta_0 \) is the equilibrium angle and \( r_1 \) and \( r_2 \) are the equilibrium bond lengths.

See (Sun) for a description of the COMPASS class2 force field.

Coefficients for the \( E_a \), \( E_{bb} \), and \( E_{ba} \) formulas must be defined for each angle type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands.

These are the 4 coefficients for the \( E_a \) formula:

- \( \theta_0 \) (degrees)
- \( K_2 \) (energy/radian^2)
- \( K_3 \) (energy/radian^3)
- \( K_4 \) (energy/radian^4)

\( \theta_0 \) is specified in degrees, but LAMMPS converts it to radians internally; hence the units of the various \( K \) are in per-radian.

For the \( E_{bb} \) formula, each line in a bond_coeff command in the input script lists 4 coefficients, the first of which is "bb" to indicate they are BondBond coefficients. In a data file, these coefficients should be listed under a "BondBond Coeffs" heading and you must leave out the "bb", i.e. only list 3 coefficients after the angle type.
For the Eba formula, each line in a bond_coeff command in the input script lists 5 coefficients, the first of which is "ba" to indicate they are BondAngle coefficients. In a data file, these coefficients should be listed under a "BondAngle Coeffs" heading and you must leave out the "ba", i.e. only list 4 coefficients after the angle type.

The theta0 value in the Eba formula is not specified, since it is the same value from the Ea formula.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the CLASS2 package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

angle_coeff command

Syntax:

angle_coeff N args

- N = angle type (see asterisk form below)
- args = coefficients for one or more angle types

Examples:

angle_coeff 1 300.0 107.0
angle_coeff * 5.0
angle_coeff 2*10 5.0

Description:

Specify the angle force field coefficients for one or more angle types. The number and meaning of the coefficients depends on the angle style. Angle coefficients can also be set in the data file read by the read_data command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple angle types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of angle types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using an angle_coeff command can override a previous setting for the same angle type. For example, these commands set the coeffs for all angle types, then overwrite the coeffs for just angle type 2:

angle_coeff * 200.0 107.0 1.2
angle_coeff 2 50.0 107.0

A line in a data file that specifies angle coefficients uses the exact same format as the arguments of the angle_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Angle Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

1 300.0 107.0

The angle_style class2 is an exception to this rule, in that an additional argument is used in the input script to allow specification of the cross-term coefficients. See its doc page for details.

Here is an alphabetic list of angle styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated angle_coeff command.

Note that there are also additional angle styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the angle section of this page.

- angle_style none - turn off angle interactions
- angle_style hybrid - define multiple styles of angle interactions
- angle_style charmm - CHARMM angle
- angle_style class2 - COMPASS (class 2) angle
- angle_style cosine - cosine angle potential
- angle_style cosine/delta - difference of cosines angle potential
- angle_style cosine/periodic - DREIDING angle
- angle_style cosine/squared - cosine squared angle potential
- angle_style harmonic - harmonic angle
- angle_style table - tabulated by angle

**Restrictions:**

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

An angle style must be defined before any angle coefficients are set, either in the input script or in a data file.

**Related commands:**

angle_style

**Default:** none
angle_style cosine command

angle_style cosine/omp command

Syntax:

angle_style cosine

Examples:

angle_style cosine
angle_coeff * 75.0

Description:

The cosine angle style uses the potential

\[ E = K [1 + \cos(\theta)] \]

where K is defined for each angle type.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:
angle_coeff

Default: none
angle_style cosine/delta command

angle_style cosine/delta/omp command

Syntax:

angle_style cosine/delta

Examples:

angle_style cosine/delta
angle_coeff 2*4 75.0 100.0

Description:

The cosine/delta angle style uses the potential

\[ E = K \left[ 1 - \cos(\theta - \theta_0) \right] \]

where theta0 is the equilibrium value of the angle, and K is a prefactor. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- theta0 (degrees)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.
Related commands:
angle_coeff, angle_style cosine/squared

Default: none
angle_style cosine/periodic command

angle_style cosine/periodic/omp command

Syntax:

angle_style cosine/periodic

Examples:

angle_style cosine/periodic
angle_coeff * 75.0 1 6

Description:

The cosine/periodic angle style uses the following potential, which is commonly used in the DREIDING force field, particularly for organometallic systems where \( n = 4 \) might be used for an octahedral complex and \( n = 3 \) might be used for a trigonal center:

\[
E = C \left[ 1 - B(-1)^n \cos(n\theta) \right]
\]

where \( C, B \) and \( n \) are coefficients defined for each angle type.

See (Mayo) for a description of the DREIDING force field

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- \( C \) (energy)
- \( B = 1 \) or \(-1\)
- \( n = 1, 2, 3, 4, 5 \) or \( 6 \) for periodicity

Note that the prefactor \( C \) is specified and not the overall force constant \( K = C / n^2 \). When \( B = 1 \), it leads to a minimum for the linear geometry. When \( B = -1 \), it leads to a maximum for the linear geometry.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.
Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

angle_style cosine/shift command

angle_style cosine/shift/omp command

Syntax:

angle_style cosine/shift

Examples:

angle_style cosine/shift
angle_coeff * 10.0 45.0

Description:

The cosine/shift angle style uses the potential

\[ E = -\frac{U_{\text{min}}}{2} \left[ 1 + \cos(\theta - \theta_0) \right] \]

where \( \theta_0 \) is the equilibrium angle. The potential is bounded between \(-U_{\text{min}}\) and zero. In the neighborhood of the minimum \( E = -U_{\text{min}} + U_{\text{min}}/4(\theta - \theta_0)^2 \) hence the spring constant is \( U_{\text{min}}/2 \).

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- \( U_{\text{min}} \) (energy)
- \( \theta \) (angle)

Styles with a \textit{cuda}, \textit{gpu}, \textit{omp}, or \textit{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:
This angle style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

**Related commands:**

angle_coeff, angle_cosineshiftexp

**Default:** none
angle_style cosine/shift/exp command

angle_style cosine/shift/exp/omp command

Syntax:

angle_style cosine/shift/exp

Examples:

angle_style cosine/shift/exp
angle_coeff * 10.0 45.0 2.0

Description:

The cosine/shift/exp angle style uses the potential

\[ E = -U_{\text{min}} \frac{e^{-aU(\theta, \theta_0)} - 1}{e^a - 1} \quad \text{with} \quad U(\theta, \theta_0) = -0.5 \left(1 + \cos(\theta - \theta_0)\right) \]

where Umin, theta, and a are defined for each angle type.

The potential is bounded between [-Umin:0] and the minimum is located at the angle theta0. The a parameter can be both positive or negative and is used to control the spring constant at the equilibrium.

The spring constant is given by \( k = A \exp(A) U_{\text{min}} / [2 (\exp(a)-1)] \). For a > 3, k/Umin = a/2 to better than 5% relative error. For negative values of the a parameter, the spring constant is essentially zero, and anharmonic terms takes over. The potential is furthermore well behaved in the limit a -> 0, where it has been implemented to linear order in a for a < 0.001. In this limit the potential reduces to the cosineshifted potential.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- umin (energy)
- theta (angle)
- A (real number)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in SectionAccelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the
-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff, angle_cosineshift, dihedral_cosineshift

Default: none
angle_style cosine/squared command

angle_style cosine/squared/omp command

Syntax:

angle_style cosine/squared

Examples:

angle_style cosine/squared
angle_coeff 2*4 75.0 100.0

Description:

The cosine/squared angle style uses the potential

\[ E = K \left[ \cos(\theta) - \cos(\theta_0) \right]^2 \]

where \( \theta_0 \) is the equilibrium value of the angle, and \( K \) is a prefactor. Note that the usual \( 1/2 \) factor is included in \( K \).

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- \( K \) (energy)
- \( \theta_0 \) (degrees)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:
This angle style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none
angle_style dipole command

angle_style dipole/omp command

Syntax:

angle_style dipole

Examples:

angle_style dipole
angle_coeff 6 2.1 180.0

Description:

The dipole angle style is used to control the orientation of a dipolar atom within a molecule (Orsi). Specifically, the dipole angle style restrains the orientation of a point dipole \( \mu_j \) (embedded in atom 'j') with respect to a reference (bond) vector \( r_{ij} = r_i - r_j \), where 'i' is another atom of the same molecule (typically, 'i' and 'j' are also covalently bonded).

It is convenient to define an angle gamma between the 'free' vector \( \mu_j \) and the reference (bond) vector \( r_{ij} \):

\[
\cos \gamma = \frac{\mu_j \cdot r_{ij}}{\mu_j \cdot r_{ij}}
\]

The dipole angle style uses the potential:

\[
E = K (\cos \gamma - \cos \gamma_0)^2
\]

where \( K \) is a rigidity constant and gamma0 is an equilibrium (reference) angle.

The torque on the dipole can be obtained by differentiating the potential using the 'chain rule' as in appendix C.3 of (Allen):

\[
\vec{T}_j = \frac{2K(\cos \gamma - \cos \gamma_0)}{\mu_j \cdot r_{ij}} \vec{r}_{ij} \times \vec{\mu}_j
\]

Example: if gamma0 is set to 0 degrees, the torque generated by the potential will tend to align the dipole along the reference direction defined by the (bond) vector \( r_{ij} \) (in other words, \( \mu_j \) is restrained to point towards atom 'i').
Note that the angle dipole potential does not give rise to any force, because it does not depend on the distance between \( i \) and \( j \) (it only depends on the angle between \( \mu_j \) and \( r_{ij} \)).

The following coefficients must be defined for each angle type via the \texttt{angle\_coeff} command as in the example above, or in the data file or restart files read by the \texttt{read\_data} or \texttt{read\_restart} commands:

- \( K \) (energy)
- \( \gamma_0 \) (degrees)

Styles with a \texttt{cuda}, \texttt{gpu}, \texttt{omp}, or \texttt{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \texttt{-suffix} command-line switch when you invoke LAMMPS, or you can use the \texttt{suffix} command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**

This angle style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

IMPORTANT NOTE: In the "Angles" section of the data file, the atom ID 'j' corresponding to the dipole to restrain must come before the atom ID of the reference atom 'i'. A third atom ID 'k' must also be provided, although 'k' is just a 'dummy' atom which can be any atom; it may be useful to choose a convention (e.g., 'k=\'i\') and adhere to it. For example, if ID=1 for the dipolar atom to restrain, and ID=2 for the reference atom, the corresponding line in the "Angles" section of the data file would read: X X 1 2 2

The "newton" command for intramolecular interactions must be "on" (which is the default).

This angle style should not be used with SHAKE.

**Related commands:**

\texttt{angle\_coeff}, \texttt{angle\_hybrid}

**Default:** none


angle_style harmonic command

angle_style harmonic/omp command

Syntax:

angle_style harmonic

Examples:

angle_style harmonic
angle_coeff 1 300.0 107.0

Description:

The **harmonic** angle style uses the potential

\[ E = K(\theta - \theta_0)^2 \]

where \( \theta_0 \) is the equilibrium value of the angle, and \( K \) is a prefactor. Note that the usual 1/2 factor is included in \( K \).

The following coefficients must be defined for each angle type via the `angle_coeff` command as in the example above, or in the data file or restart files read by the `read_data` or `read_restart` commands:

- \( K \) (energy/radian^2)
- \( \theta_0 \) (degrees)

\( \theta_0 \) is specified in degrees, but LAMMPS converts it to radians internally; hence the units of \( K \) are in energy/radian^2.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions: none
This angle style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none
angle_style hybrid command

Syntax:

angle_style hybrid style1 style2 ...

- style1,style2 = list of one or more angle styles

Examples:

angle_style hybrid harmonic cosine
angle_coeff 1 harmonic 80.0 30.0
angle_coeff 2* cosine 50.0

Description:

The hybrid style enables the use of multiple angle styles in one simulation. An angle style is assigned to each angle type. For example, angles in a polymer flow (of angle type 1) could be computed with a harmonic potential and angles in the wall boundary (of angle type 2) could be computed with a cosine potential. The assignment of angle type to style is made via the angle_coeff command or in the data file.

In the angle_coeff commands, the name of an angle style must be added after the angle type, with the remaining coefficients being those appropriate to that style. In the example above, the 2 angle_coeff commands set angles of angle type 1 to be computed with a harmonic potential with coefficients 80.0, 30.0 for K, theta0. All other angle types (2-N) are computed with a cosine potential with coefficient 50.0 for K.

If angle coefficients are specified in the data file read via the read_data command, then the same rule applies. E.g. "harmonic" or "cosine", must be added after the angle type, for each line in the "Angle Coefs" section, e.g.

Angle Coefs

1 harmonic 80.0 30.0
2 cosine 50.0
...

If class2 is one of the angle hybrid styles, the same rule holds for specifying additional BondBond (and BondAngle) coefficients either via the input script or in the data file. I.e. class2 must be added to each line after the angle type. For lines in the BondBond (or BondAngle) section of the data file for angle types that are not class2, you must use an angle style of skip as a placeholder, e.g.

BondBond Coefs

1 skip
2 class2 3.6512 1.0119 1.0119
...

Note that it is not necessary to use the angle style skip in the input script, since BondBond (or BondAngle) coefficients need not be specified at all for angle types that are not class2.

An angle style of none with no additional coefficients can be used in place of an angle style, either in a input script angle_coeff command or in the data file, if you desire to turn off interactions for specific angle types.
**Restrictions:**

This angle style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the [Making LAMMPS] section for more info on packages.

Unlike other angle styles, the hybrid angle style does not store angle coefficient info for individual sub-styles in a binary restart files. Thus when restarting a simulation from a restart file, you need to re-specify angle_coeff commands.

**Related commands:**

angle_coeff

**Default:** none
angle_style none command

Syntax:

angle_style none

Examples:

angle_style none

Description:

Using an angle style of none means angle forces are not computed, even if triplets of angle atoms were listed in the data file read by the read_data command.

Restrictions: none

Related commands: none

Default: none
angle_style sdk command

Syntax:

angle_style sdk

angle_style sdk/omp

Examples:

angle_style sdk
angle_coeff 1 300.0 107.0

Description:

The sdk angle style is a combination of the harmonic angle potential,

\[ E = K(\theta - \theta_0)^2 \]

where \( \theta_0 \) is the equilibrium value of the angle and \( K \) a prefactor, with the repulsive part of the non-bonded \( \text{lj/sdk} \) pair style between the atoms 1 and 3. This angle potential is intended for coarse grained MD simulations with the CMM parametrization using the pair_style \( \text{lj/sdk} \). Relative to the pair_style \( \text{lj/sdk} \), however, the energy is shifted by \( \epsilon \), to avoid sudden jumps. Note that the usual 1/2 factor is included in \( K \).

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above:

- \( K \) (energy/radian^2)
- \( \theta_0 \) (degrees)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of \( K \) are in energy/radian^2. The also required \( \text{lj/sdk} \) parameters will be extracted automatically from the pair_style.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER-CG-CMM package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff, angle_style harmonic, pair_style \( \text{lj/sdk} \), pair_style \( \text{lj/sdk/coul/long} \)

Default: none
angle_style command

Syntax:

angle_style style

- style = none or hybrid or charmm or class2 or cosine or cosine/squared or harmonic

Examples:

angle_style harmonic
angle_style charmm
angle_style hybrid harmonic cosine

Description:

Set the formula(s) LAMMPS uses to compute angle interactions between triplets of atoms, which remain in force for the duration of the simulation. The list of angle triplets is read in by a read_data or read_restart command from a data or restart file.

Hybrid models where angles are computed using different angle potentials can be setup using the hybrid angle style.

The coefficients associated with a angle style can be specified in a data or restart file or via the angle_coeff command.

All angle potentials store their coefficient data in binary restart files which means angle_style and angle_coeff commands do not need to be re-specified in an input script that restarts a simulation. See the read_restart command for details on how to do this. The one exception is that angle_style hybrid only stores the list of sub-styles in the restart file; angle coefficients need to be re-specified.

IMPORTANT NOTE: When both an angle and pair style is defined, the special_bonds command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between 3 bonded atoms.

In the formulas listed for each angle style, \( theta \) is the angle between the 3 atoms in the angle.

Here is an alphabetic list of angle styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated angle_coeff command.

Note that there are also additional angle styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the angle section of this page.
- **angle_style harmonic** - harmonic angle
- **angle_style table** - tabulated by angle

**Restrictions:**

Angle styles can only be set for atom_styles that allow angles to be defined.

Most angle styles are part of the MOLECULAR package. They are only enabled if LAMMPS was built with that package. See the [Making LAMMPS](#) section for more info on packages. The doc pages for individual bond potentials tell if it is part of a package.

**Related commands:**

angle_coeff

**Default:**

angle_style none
angle_style table command

angle_style table/omp command

Syntax:

angle_style table style N

- style = *linear* or *spline* = method of interpolation
- N = use N values in table

Examples:

angle_style table linear 1000
angle_coeff 3 file.table ENTRY1

Description:

Style *table* creates interpolation tables of length *N* from angle potential and derivative values listed in a file(s) as a function of angle. The files are read by the *angle_coeff* command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and derivative values at each of *N* angles. During a simulation, these tables are used to interpolate energy and force values on individual atoms as needed. The interpolation is done in one of 2 styles: *linear* or *spline*.

For the *linear* style, the angle is used to find 2 surrounding table values from which an energy or its derivative is computed by linear interpolation.

For the *spline* style, a cubic spline coefficients are computed and stored at each of the *N* values in the table. The angle is used to find the appropriate set of coefficients which are used to evaluate a cubic polynomial which computes the energy or derivative.

The following coefficients must be defined for each angle type via the *angle_coeff* command as in the example above.

- filename
- keyword

The filename specifies a file containing tabulated energy and derivative values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# Angle potential for harmonic (one or more comment or blank lines)

HAM
N 181 FP 0 0 EQ 90.0  
N 181 FP 0 0
1 0.0 200.5 2.5
2 1.0 198.0 2.5
...  
```

(keyword is the first text on line)

(N, FP, EQ parameters)

(blank line)

(N, FP parameters)

(index, angle, energy, derivative)
A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the angle_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the \( N \) specified in the angle_style table command. Let Ntable = \( N \) in the angle_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and derivative values at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and force for individual angles and their atoms. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile.

The "FP" parameter is optional. If used, it is followed by two values fplo and fphi, which are the 2nd derivatives at the innermost and outermost angle settings. These values are needed by the spline construction routines. If not specified by the "FP" parameter, they are estimated (less accurately) by the first two and last two derivative values in the table.

The "EQ" parameter is also optional. If used, it is followed by a the equilibrium angle value, which is used, for example, by the fix shake command. If not used, the equilibrium angle is set to 180.0.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the angle value (in degrees), the 3rd value is the energy (in energy units), and the 4th is \(-\frac{dE}{d(\theta)}\) (also in energy units). The 3rd term is the energy of the 3-atom configuration for the specified angle. The last term is the derivative of the energy with respect to the angle (in degrees, not radians). Thus the units of the last term are still energy, not force. The angle values must increase from one line to the next. The angle values must also begin with 0.0 and end with 180.0, i.e. span the full range of possible angles.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:
This angle style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none
atom_modify command

Syntax:

```
atom_modify keyword values ...
```

- one or more keyword/value pairs may be appended
- keyword = map or first or sort

```
map value = array or hash
first value = group-ID = group whose atoms will appear first in internal atom lists
sort values = Nfreq binsize
    Nfreq = sort atoms spatially every this many time steps
    binsize = bin size for spatial sorting (distance units)
```

Examples:

```
atom_modify map hash
atom_modify map array sort 10000 2.0
atom_modify first colloid
```

Description:

Modify properties of the atom style selected within LAMMPS.

The map keyword determines how atom ID lookup is done for molecular problems. Lookups are performed by bond (angle, etc) routines in LAMMPS to find the local atom index associated with a global atom ID. When the array value is used, each processor stores a lookup table of length N, where N is the total # of atoms in the system. This is the fastest method for most simulations, but a processor can run out of memory to store the table for very large simulations. The hash value uses a hash table to perform the lookups. This method can be slightly slower than the array method, but its memory cost is proportional to N/P on each processor, where P is the total number of processors running the simulation.

The first keyword allows a group to be specified whose atoms will be maintained as the first atoms in each processor's list of owned atoms. This in only useful when the specified group is a small fraction of all the atoms, and there are other operations LAMMPS is performing that will be sped-up significantly by being able to loop over the smaller set of atoms. Otherwise the reordering required by this option will be a net slow-down. The neigh_modify include and communicate group commands are two examples of commands that require this setting to work efficiently. Several fixes, most notably time integration fixes like fix nve, also take advantage of this setting if the group they operate on is the group specified by this command. Note that specifying "all" as the group-ID effectively turns off the first option.

It is OK to use the first keyword with a group that has not yet been defined, e.g. to use the atom_modify first command at the beginning of your input script. LAMMPS does not use the group until a simulation is run.

The sort keyword turns on a spatial sorting or reordering of atoms within each processor's sub-domain every Nfreq timesteps. If Nfreq is set to 0, then sorting is turned off. Sorting can improve cache performance and thus speed-up a LAMMPS simulation, as discussed in a paper by (Meloni). Its efficacy depends on the problem size (atoms/processor), how quickly the system becomes disordered, and various other factors. As a general rule, sorting is typically more effective at speeding up simulations of liquids as opposed to solids. In tests we have done, the speed-up can range from zero to 3-4x.
Reordering is performed every $N_{freq}$ timesteps during a dynamics run or iterations during a minimization. More precisely, reordering occurs at the first reneighboring that occurs after the target timestep. The reordering is performed locally by each processor, using bins of the specified $binsize$. If $binsize$ is set to 0.0, then a $binsize$ equal to half the neighbor cutoff distance (force cutoff plus skin distance) is used, which is a reasonable value. After the atoms have been binned, they are reordered so that atoms in the same bin are adjacent to each other in the processor’s 1d list of atoms.

The goal of this procedure is for atoms to put atoms close to each other in the processor's one-dimensional list of atoms that are also near to each other spatially. This can improve cache performance when pairwise interactions and neighbor lists are computed. Note that if bins are too small, there will be few atoms/bin. Likewise if bins are too large, there will be many atoms/bin. In both cases, the goal of cache locality will be undermined.

IMPORTANT NOTE: Running a simulation with sorting on versus off should not change the simulation results in a statistical sense. However, a different ordering will induce round-off differences, which will lead to diverging trajectories over time when comparing two simulations. Various commands, particularly those which use random numbers (e.g. velocity create, and fix langevin), may generate (statistically identical) results which depend on the order in which atoms are processed. The order of atoms in a dump file will also typically change if sorting is enabled.

**Restrictions:**

The map keyword can only be used before the simulation box is defined by a read_data or create_box command.

The first and sort options cannot be used together. Since sorting is on by default, it will be turned off if the first keyword is used with a group-ID that is not "all".

**Related commands:** none

**Default:**

By default, atomic (non-molecular) problems do not allocate maps. For molecular problems, the option default is map = array. By default, a "first" group is not defined. By default, sorting is enabled with a frequency of 1000 and a $binsize$ of 0.0, which means the neighbor cutoff will be used to set the bin size.

atom_style command

Syntax:

atom_style style args

- style = angle or atomic or bond or charge or dipole or electron or ellipsoid or full or line or meso or molecular or peri or sphere or tri or hybrid

args = none for any style except hybrid
hybrid args = list of one or more sub-styles

Examples:

atom_style atomic
atom_style bond
atom_style full
atom_style hybrid charge bond

Description:

Define what style of atoms to use in a simulation. This determines what attributes are associated with the atoms. This command must be used before a simulation is setup via a read_data, read_restart, or create_box command.

Once a style is assigned, it cannot be changed, so use a style general enough to encompass all attributes. E.g. with style bond, angular terms cannot be used or added later to the model. It is OK to use a style more general than needed, though it may be slightly inefficient.

The choice of style affects what quantities are stored by each atom, what quantities are communicated between processors to enable forces to be computed, and what quantities are listed in the data file read by the read_data command.

These are the additional attributes of each style and the typical kinds of physical systems they are used to model. All styles store coordinates, velocities, atom IDs and types. See the read_data, create_atoms, and set commands for info on how to set these various quantities.

<table>
<thead>
<tr>
<th>style</th>
<th>attributes</th>
<th>typical systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>angle</td>
<td>bonds and angles</td>
<td>bead-spring polymers with stiffness</td>
</tr>
<tr>
<td>atomic</td>
<td>only the default values</td>
<td>coarse-grain liquids, solids, metals</td>
</tr>
<tr>
<td>bond</td>
<td>bonds</td>
<td>bead-spring polymers</td>
</tr>
<tr>
<td>charge</td>
<td>charge</td>
<td>atomic system with charges</td>
</tr>
<tr>
<td>dipole</td>
<td>charge and dipole moment</td>
<td>system with dipolar particles</td>
</tr>
<tr>
<td>electron</td>
<td>charge and spin and eradius</td>
<td>electronic force field</td>
</tr>
<tr>
<td>ellipsoid</td>
<td>shape, quaternion for particle orientation, angular momentum</td>
<td>extended aspherical particles</td>
</tr>
<tr>
<td>full</td>
<td>molecular + charge</td>
<td>bio-molecules</td>
</tr>
<tr>
<td>line</td>
<td>end points, angular velocity</td>
<td>rigid bodies</td>
</tr>
<tr>
<td>meso</td>
<td>rho, e, cv</td>
<td>SPH particles</td>
</tr>
<tr>
<td>molecular</td>
<td>bonds, angles, dihedrals, impropers</td>
<td>uncharged molecules</td>
</tr>
<tr>
<td>peri</td>
<td>mass, volume</td>
<td>mesoscopic Peridynamic models</td>
</tr>
</tbody>
</table>
All of the styles assign mass to particles on a per-type basis, using the `mass` command, except for the finite-size particle styles discussed below. They assign mass on a per-atom basis.

All of the styles define point particles, except the `sphere`, `ellipsoid`, `electron`, `peri`, `wavepacket`, `line`, and `tri` styles, which define finite-size particles.

For the `sphere` style, the particles are spheres and each stores a per-particle diameter and mass. If the diameter > 0.0, the particle is a finite-size sphere. If the diameter = 0.0, it is a point particle.

For the `ellipsoid` style, the particles are ellipsoids and each stores a flag which indicates whether it is a finite-size ellipsoid or a point particle. If it is an ellipsoid, it also stores a shape vector with the 3 diameters of the ellipsoid and a quaternion 4-vector with its orientation.

For the `electron` style, the particles representing electrons are 3d Gaussians with a specified position and bandwidth or uncertainty in position, which is represented by the `eradius = electron size`.

For the `peri` style, the particles are spherical and each stores a per-particle mass and volume.

The `meso` style is for smoothed particle hydrodynamics (SPH) particles which store a density (rho), energy (e), and heat capacity (cv).

The `wavepacket` style is similar to `electron`, but the electrons may consist of several Gaussian wave packets, summed up with coefficients `cs = (cs_re,cs_im)`. Each of the wave packets is treated as a separate particle in LAMMPS, wave packets belonging to the same electron must have identical `etag` values.

For the `line` style, the particles are idealized line segments and each stores a per-particle mass and length and orientation (i.e. the end points of the line segment).

For the `tri` style, the particles are planar triangles and each stores a per-particle mass and size and orientation (i.e. the corner points of the triangle).

Typically, simulations require only a single (non-hybrid) atom style. If some atoms in the simulation do not have all the properties defined by a particular style, use the simplest style that defines all the needed properties by any atom. For example, if some atoms in a simulation are charged, but others are not, use the `charge` style. If some atoms have bonds, but others do not, use the `bond` style.

The only scenario where the `hybrid` style is needed is if there is no single style which defines all needed properties of all atoms. For example, if you want dipolar particles which will be torqued and rotate, you would need to use "atom_style hybrid sphere dipole". When a hybrid style is used, atoms store and communicate the union of all quantities implied by the individual styles.

LAMMPS can be extended with new atom styles; see this section.

Restrictions:

This command cannot be used after the simulation box is defined by a `read_data` or `create_box` command.

The `angle`, `bond`, `full`, and `molecular` styles are part of the MOLECULAR package. The `dipole` style is part of the "dipole" package. The `peri` style is part of the PERI package for Peridynamics. The `electron` style is part of the
USER-EFF package for electronic force fields. The \textit{meso} style is part of the USER-SPH package for smoothed particle hydrodynamics (SPH). See this PDF guide to using SPH in LAMMPS. The \textit{wavepacket} style is part of the USER-AWPMD package for the antisymmetrized wave packet MD method. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

\textbf{Related commands:}

read\_data, pair\_style

\textbf{Default:}

atom\_style atomic
balance command

Syntax:

balance keyword args ...

- one or more keyword/arg pairs may be appended
- keyword = x or y or z or dynamic or out

  
x args = uniform or Px-1 numbers between 0 and 1
  uniform = evenly spaced cuts between processors in x dimension
  numbers = Px-1 ascending values between 0 and 1, Px - # of processors in x dimension
  y args = uniform or Py-1 numbers between 0 and 1
  uniform = evenly spaced cuts between processors in y dimension
  numbers = Py-1 ascending values between 0 and 1, Py - # of processors in y dimension
  z args = uniform or Pz-1 numbers between 0 and 1
  uniform = evenly spaced cuts between processors in z dimension
  numbers = Pz-1 ascending values between 0 and 1, Pz - # of processors in z dimension
  dynamic args = dimstr Niter thresh
  dimstr = sequence of letters containing "x" or "y" or "z", each not more than once
  Niter = # of times to iterate within each dimension of dimstr sequence
  thresh = stop balancing when this imbalance threshold is reached
  out arg = filename
  filename = output file to write each processor's sub-domain to

Examples:

balance x uniform y 0.4 0.5 0.6
balance dynamic xz 5 1.1
balance dynamic x 20 1.0 out tmp.balance

Description:

This command adjusts the size of processor sub-domains within the simulation box, to attempt to balance the number of particles and thus the computational cost (load) evenly across processors. The load balancing is "static" in the sense that this command performs the balancing once, before or between simulations. The processor sub-domains will then remain static during the subsequent run. To perform "dynamic" balancing, see the fix balance command, which can adjust processor sub-domain sizes on-the-fly during a run.

Load-balancing is only useful if the particles in the simulation box have a spatially-varying density distribution. E.g. a model of a vapor/liquid interface, or a solid with an irregular-shaped geometry containing void regions. In this case, the LAMMPS default of dividing the simulation box volume into a regular-spaced grid of processor sub-domain, with one equal-volume sub-domain per processor, may assign very different numbers of particles per processor. This can lead to poor performance in a scalability sense, when the simulation is run in parallel.

Note that the processors command gives you control over how the box volume is split across processors. Specifically, for a Px by Py by Pz grid of processors, it chooses or lets you choose Px, Py, and Pz, subject to the constraint that Px * Py * Pz = P, the total number of processors. This is sufficient to achieve good load-balance for many models on many processor counts. However, all the processor sub-domains will still be the same shape and have the same volume.

This command does not alter the topology of the Px by Py by Pz grid or processors. But it shifts the cutting planes between processors (in 3d, or lines in 2d), which adjusts the volume (area in 2d) assigned to each processor, as in
the following 2d diagram. The left diagram is the default partitioning of the simulation box across processors (one sub-box for each of 16 processors); the right diagram is after balancing.

When the balance command completes, it prints out the final positions of all cutting planes in each of the 3 dimensions (as fractions of the box length). It also prints statistics about its results, including the change in "imbalance factor". This factor is defined as the maximum number of particles owned by any processor, divided by the average number of particles per processor. Thus an imbalance factor of 1.0 is perfect balance. For 10000 particles running on 10 processors, if the most heavily loaded processor has 1200 particles, then the factor is 1.2, meaning there is a 20% imbalance. The change in the maximum number of particles (on any processor) is also printed.

IMPORTANT NOTE: This command attempts to minimize the imbalance factor, as defined above. But because of the topology constraint that only the cutting planes (lines) between processors are moved, there are many irregular distributions of particles, where this factor cannot be shrunk to 1.0, particularly in 3d. Also, computational cost is not strictly proportional to particle count, and changing the relative size and shape of processor sub-domains may lead to additional computational and communication overheads, e.g. in the PPPM solver used via the kspace_style command. Thus you should benchmark the run times of your simulation before and after balancing.

The \textit{x}, \textit{y}, and \textit{z} keywords adjust the position of cutting planes between processor sub-domains in a specific dimension. The \textit{uniform} argument spaces the planes evenly, as in the left diagram above. The \textit{numeric} argument requires you to list \(P_s-1\) numbers that specify the position of the cutting planes. This requires that you know \(P_s = P_x \) or \( P_y \) or \( P_z = \) the number of processors assigned by LAMMPS to the relevant dimension. This assignment is made (and the \( P_x, P_y, P_z \) values printed out) when the simulation box is created by the "create_box" or "read_data" or "read_restart" command and is influenced by the settings of the "processors" command.

Each of the numeric values must be between 0 and 1, and they must be listed in ascending order. They represent the fractional position of the cutting place. The left (or lower) edge of the box is 0.0, and the right (or upper) edge is 1.0. Neither of these values is specified. Only the interior \(P_s-1\) positions are specified. Thus if there are 2 processors in the \textit{x} dimension, you specify a single value such as 0.75, which would make the left processor's sub-domain 3x larger than the right processor's sub-domain.

The \textit{dynamic} keyword changes the cutting planes between processors in an iterative fashion, seeking to reduce the imbalance factor, similar to how the \textbf{fix balance} command operates. Note that this keyword begins its operation from the current processor partitioning, which could be uniform or the result of a previous balance command.

The \textit{dimstr} argument is a string of characters, each of which must be an "x" or "y" or "z". Each character can
appear zero or one time, since there is no advantage to balancing on a dimension more than once. You should normally only list dimensions where you expect there to be a density variation in the particles.

Balancing proceeds by adjusting the cutting planes in each of the dimensions listed in \textit{dimstr}, one dimension at a time. For a single dimension, the balancing operation (described below) is iterated on up to \textit{Niter} times. After each dimension finishes, the imbalance factor is re-computed, and the balancing operation halts if the \textit{thresh} criterion is met.

A rebalance operation in a single dimension is performed using a recursive multisectioning algorithm, where the position of each cutting plane (line in 2d) in the dimension is adjusted independently. This is similar to a recursive bisectioning (RCB) for a single value, except that the bounds used for each bisectioning take advantage of information from neighboring cuts if possible. At each iteration, the count of particles on either side of each plane is tallied. If the counts do not match the target value for the plane, the position of the cut is adjusted to be halfway between a low and high bound. The low and high bounds are adjusted on each iteration, using new count information, so that they become closer together over time. Thus as the recursion progresses, the count of particles on either side of the plane gets closer to the target value.

Once the rebalancing is complete and final processor sub-domains assigned, particles are migrated to their new owning processor, and the balance procedure ends.

IMPORTANT NOTE: At each rebalance operation, the RCB for each cutting plane (line in 2d) typically starts with low and high bounds separated by the extent of a processor's sub-domain in one dimension. The size of this bracketing region shrinks by 1/2 every iteration. Thus if \textit{Niter} is specified as 10, the cutting plane will typically be positioned to 1 part in 1000 accuracy (relative to the perfect target position). For \textit{Niter} = 20, it will be accurate to 1 part in a million. Thus there is no need to set \textit{Niter} to a large value. LAMMPS will check if the threshold accuracy is reached (in a dimension) is less iterations than \textit{Niter} and exit early. However, \textit{Niter} should also not be set too small, since it will take roughly the same number of iterations to converge even if the cutting plane is initially close to the target value.

IMPORTANT NOTE: If a portion of your system is a perfect lattice, e.g. the initial system is generated by the \texttt{create_atoms} command, then the balancer may be unable to achieve exact balance. I.e. entire lattice planes will be owned or not owned by a single processor. So you should not expect to achieve perfect balance in this case.

The \texttt{out} keyword writes a text file to the specified \textit{filename} with the results of the balancing operation. The file contains the bounds of the sub-domain for each processor after the balancing operation completes. The format of the file is compatible with the \texttt{Pizza.py mdump} tool which has support for manipulating and visualizing mesh files. An example is shown here for a balancing by 4 processors for a 2d problem:

```plaintext
ITEM: TIMESTEP
0
ITEM: NUMBER OF SQUARES
4
ITEM: SQUARES
1 1 1 2 7 6
2 2 2 3 8 7
3 3 3 4 9 8
4 4 4 5 10 9
ITEM: TIMESTEP
0
ITEM: NUMBER OF NODES
10
ITEM: BOX BOUNDS
-153.919 184.703
0 15.3919
-0.769595 0.769595
ITEM: NODES
```
The "SQUARES" lists the node IDs of the 4 vertices in a rectangle for each processor (1 to 4). The first SQUARE 1 (for processor 0) is a rectangle of type 1 (equal to SQUARE ID) and contains vertices 1,2,7,6. The coordinates of all the vertices are listed in the NODES section. Note that the 4 sub-domains share vertices, so there are only 10 unique vertices in total.

For a 3d problem, the syntax is similar with "SQUARES" replaced by "CUBES", and 8 vertices listed for each processor, instead of 4.

**Restrictions:**

The *dynamic* keyword cannot be used with the *x*, *y*, or *z* arguments.

For 2d simulations, the *z* keyword cannot be used. Nor can a "z" appear in *dimstr* for the *dynamic* keyword.

**Related commands:**

processors, fix balance

**Default:** none
bond_style class2 command

bond_style class2/omp command

Syntax:

bond_style class2

Examples:

bond_style class2
bond_coeff 1 1.0 100.0 80.0 80.0

Description:

The class2 bond style uses the potential

\[ E = K_2(r - r_0)^2 + K_3(r - r_0)^3 + K_4(r - r_0)^4 \]

where \( r_0 \) is the equilibrium bond distance.

See (Sun) for a description of the COMPASS class2 force field.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- R0 (distance)
- K2 (energy/distance^2)
- K3 (energy/distance^3)
- K4 (energy/distance^4)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:
This bond style can only be used if LAMMPS was built with the CLASS2 package. See the Making LAMMPS section for more info on packages.

**Related commands:**

bond_coeff, delete_bonds

**Default:** none

---

bond_coeff command

Syntax:

bond_coeff N args

- N = bond type (see asterisk form below)
- args = coefficients for one or more bond types

Examples:

bond_coeff 5 80.0 1.2
bond_coeff * 30.0 1.5 1.0 1.0
bond_coeff 1*4 30.0 1.5 1.0 1.0
bond_coeff 1 harmonic 200.0 1.0

Description:

Specify the bond force field coefficients for one or more bond types. The number and meaning of the coefficients depends on the bond style. Bond coefficients can also be set in the data file read by the read_data command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple bond types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of bond types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using a bond_coeff command can override a previous setting for the same bond type. For example, these commands set the coeffs for all bond types, then overwrite the coeffs for just bond type 2:

bond_coeff * 100.0 1.2
bond_coeff 2 200.0 1.2

A line in a data file that specifies bond coefficients uses the exact same format as the arguments of the bond_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Bond Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

5 80.0 1.2

Here is an alphabetic list of bond styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated bond_coeff command.

Note that here are also additional bond styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the bond section of this page.

- bond_style none - turn off bonded interactions
- bond_style hybrid - define multiple styles of bond interactions
- bond_style class2 - COMPASS (class 2) bond
- **bond_style fene** - FENE (finite-extensible non-linear elastic) bond
- **bond_style fene/expand** - FENE bonds with variable size particles
- **bond_style harmonic** - harmonic bond
- **bond_style morse** - Morse bond
- **bond_style nonlinear** - nonlinear bond
- **bond_style quartic** - breakable quartic bond
- **bond_style table** - tabulated by bond length

**Restrictions:**

This command must come after the simulation box is defined by a `read_data`, `read_restart`, or `create_box` command.

A bond style must be defined before any bond coefficients are set, either in the input script or in a data file.

**Related commands:**

`bond_style`

**Default:** none
bond_style fene command

bond_style fene/omp command

Syntax:

bond_style fene

Examples:

bond_style fene
bond_coeff 1 30.0 1.5 1.0 1.0

Description:

The fene bond style uses the potential

\[ E = -0.5KR_0^2 \ln \left[ 1 - \left( \frac{r}{R_0} \right)^2 \right] + 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] + \epsilon \]

to define a finite extensible nonlinear elastic (FENE) potential (Kremer), used for bead-spring polymer models. The first term is attractive, the 2nd Lennard-Jones term is repulsive. The first term extends to R0, the maximum extent of the bond. The 2nd term is cutoff at 2^{1/6} sigma, the minimum of the LJ potential.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^2)
- R0 (distance)
- epsilon (energy)
- sigma (distance)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.
Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

You typically should specify special_bonds fene or special_bonds lj/coul 0 1 1 to use this bond style. LAMMPS will issue a warning if that's not the case.

Related commands:

bond_coeff, delete_bonds

Default: none

bond_style fene/expand command

bond_style fene/expand/omp command

Syntax:

bond_style fene/expand

Examples:

bond_style fene/expand
bond_coeff 1 30.0 1.5 1.0 1.0 0.5

Description:

The fene/expand bond style uses the potential

\[ E = -0.5K R_0^2 \ln \left[ 1 - \left( \frac{r - \Delta}{R_0} \right)^2 \right] + 4\epsilon \left[ \left( \frac{\sigma}{r - \Delta} \right)^{12} - \left( \frac{\sigma}{r - \Delta} \right)^6 \right] + \]

to define a finite extensible nonlinear elastic (FENE) potential (Kremer), used for bead-spring polymer models. The first term is attractive, the 2nd Lennard-Jones term is repulsive.

The fene/expand bond style is similar to fene except that an extra shift factor of delta (positive or negative) is added to \( r \) to effectively change the bead size of the bonded atoms. The first term now extends to \( R_0 + \delta \) and the 2nd term is cutoff at \( 2^{\frac{2}{3}} \sigma + \delta \).

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- \( K \) (energy/distance^2)
- \( R_0 \) (distance)
- epsilon (energy)
- sigma (distance)
- delta (distance)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.
You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

You typically should specify special_bonds fene or special_bonds lj/coul 0 1 1 to use this bond style. LAMMPS will issue a warning it that's not the case.

Related commands:

bond_coeff, delete_bonds

Default: none

bond_style harmonic command

bond_style harmonic/omp command

Syntax:

bond_style harmonic

Examples:

bond_style harmonic
bond_coeff 5 80.0 1.2

Description:

The harmonic bond style uses the potential

\[ E = K(r - r_0)^2 \]

where \( r_0 \) is the equilibrium bond distance. Note that the usual \( 1/2 \) factor is included in \( K \).

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- \( K \) (energy/distance^2)
- \( r_0 \) (distance)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:
bond_coeff, delete_bonds

Default: none
**bond_style harmonic/shift command**

**bond_style harmonic/shift/omp command**

**Syntax:**

\[ \text{bond_style harmonic/shift} \]

**Examples:**

\[ \text{bond_style harmonic/shift} \]
\[ \text{bond_coeff 5 10.0 0.5 1.0} \]

**Description:**

The `harmonic/shift` bond style is a shifted harmonic bond that uses the potential

\[ E = \frac{U_{\text{min}}}{(r_0 - r_c)^2} \left[ (r - r_0)^2 - (r_c - r_0)^2 \right] \]

where \( r_0 \) is the equilibrium bond distance, and \( r_c \) the critical distance. The potential is \(-U_{\text{min}}\) at \( r_0 \) and zero at \( r_c \). The spring constant is \( k = U_{\text{min}} / [2 (r_0-r_c)^2] \).

The following coefficients must be defined for each bond type via the `bond_coeff` command as in the example above, or in the data file or restart files read by the `read_data` or `read_restart` commands:

- \( U_{\text{min}} \) (energy)
- \( r_0 \) (distance)
- \( r_c \) (distance)

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**
This bond style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

**Related commands:**

`bond_coeff`, `delete_bonds`, `bond_harmonic`

**Default:** none
bond_style harmonic/shift/cut command

bond_style harmonic/shift/cut/omp command

Syntax:

bond_style harmonic/shift/cut

Examples:

bond_style harmonic/shift/cut
bond_coeff 5 10.0 0.5 1.0

Description:

The harmonic/shift/cut bond style is a shifted harmonic bond that uses the potential

\[ E = \frac{U_{\text{min}}}{(r_0 - r_c)^2} \left[ (r - r_0)^2 - (r_c - r_0)^2 \right] \]

where \( r_0 \) is the equilibrium bond distance, and \( r_c \) the critical distance. The bond potential is zero for distances \( r > r_c \). The potential is \(-U_{\text{min}}\) at \( r_0 \) and zero at \( r_c \). The spring constant is \( k = U_{\text{min}} / [2 (r_0-r_c)^2] \).

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- \( U_{\text{min}} \) (energy)
- \( r_0 \) (distance)
- \( r_c \) (distance)

Styles with a \( \text{cuda} \), \( \text{gpu} \), \( \text{omp} \), or \( \text{opt} \) suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:
This bond style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

**Related commands:**

bond_coeff, delete_bonds, bond_harmonic, bond_harmonicshift

**Default:** none
**bond_style hybrid command**

**Syntax:**

```
bond_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more bond styles

**Examples:**

```
bond_style hybrid harmonic fene
bond_coeff 1 harmonic 80.0 1.2
bond_coeff 2 fene 30.0 1.5 1.0 1.0
```

**Description:**

The hybrid style enables the use of multiple bond styles in one simulation. A bond style is assigned to each bond type. For example, bonds in a polymer flow (of bond type 1) could be computed with a fene potential and bonds in the wall boundary (of bond type 2) could be computed with a harmonic potential. The assignment of bond type to style is made via the bond_coeff command or in the data file.

In the bond_coeff commands, the name of a bond style must be added after the bond type, with the remaining coefficients being those appropriate to that style. In the example above, the 2 bond_coeff commands set bonds of bond type 1 to be computed with a harmonic potential with coefficients 80.0, 1.2 for K, r0. All other bond types (2-N) are computed with a fene potential with coefficients 30.0, 1.5, 1.0, 1.0 for K, R0, epsilon, sigma.

If bond coefficients are specified in the data file read via the read_data command, then the same rule applies. E.g. "harmonic" or "fene" must be added after the bond type, for each line in the "Bond Coeffs" section, e.g.

```
Bond Coeffs

1 harmonic 80.0 1.2
2 fene 30.0 1.5 1.0 1.0
...
```

A bond style of none with no additional coefficients can be used in place of a bond style, either in an input script bond_coeff command or in the data file, if you desire to turn off interactions for specific bond types.

**Restrictions:**

This bond style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Unlike other bond styles, the hybrid bond style does not store bond coefficient info for individual sub-styles in a binary restart files. Thus when restarting a simulation from a restart file, you need to re-specify bond_coeff commands.

**Related commands:**

bond_coeff, delete_bonds
Default: none
bond_style morse command

bond_style morse/omp command

Syntax:

bond_style morse

Examples:

bond_style morse
bond_coeff 5 1.0 2.0 1.2

Description:

The morse bond style uses the potential

\[ E = D \left[ 1 - e^{-\alpha(r-r_0)} \right]^2 \]

where \( r_0 \) is the equilibrium bond distance, alpha is a stiffness parameter, and D determines the depth of the potential well.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- D (energy)
- alpha (inverse distance)
- r0 (distance)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.
Related commands:
bond_coeff, delete_bonds

Default: none
bond_style none command

Syntax:

bond_style none

Examples:

bond_style none

Description:

Using a bond style of none means bond forces are not computed, even if pairs of bonded atoms were listed in the data file read by the read_data command.

Restrictions: none

Related commands: none

Default: none
bond_style nonlinear command

bond_style nonlinear/omp command

Syntax:

bond_style nonlinear

Examples:

bond_style nonlinear
bond_coeff 2 100.0 1.1 1.4

Description:

The nonlinear bond style uses the potential

$$E = \frac{\epsilon (r - r_0)^2}{\lambda^2 - (r - r_0)^2}$$

to define an anharmonic spring (Rector) of equilibrium length $r_0$ and maximum extension $\lambda$.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- epsilon (energy)
- $r_0$ (distance)
- $\lambda$ (distance)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.
Related commands:

bond_coeff, delete_bonds

Default: none

(Rector) Rector, Van Swol, Henderson, Molecular Physics, 82, 1009 (1994).
bond_style quartic command

bond_style quartic/omp command

Syntax:

bond_style quartic

Examples:

bond_style quartic
bond_coeff 2 1200 -0.55 0.25 1.3 34.6878

Description:

The **quartic** bond style uses the potential

\[
E = K (r - R_c)^2 (r - R_c - B_1)(r - R_c - B_2) + U_0 + 4 \epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] +
\]

to define a bond that can be broken as the simulation proceeds (e.g. due to a polymer being stretched). The sigma and epsilon used in the LJ portion of the formula are both set equal to 1.0 by LAMMPS.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^2)
- B1 (distance)
- B2 (distance)
- Rc (distance)
- U0 (energy)

This potential was constructed to mimic the FENE bond potential for coarse-grained polymer chains. When monomers with sigma = epsilon = 1.0 are used, the following choice of parameters gives a quartic potential that looks nearly like the FENE potential: K = 1200, B1 = -0.55, B2 = 0.25, Rc = 1.3, and U0 = 34.6878. Different parameters can be specified using the bond_coeff command, but you will need to choose them carefully so they form a suitable bond potential.

Rc is the cutoff length at which the bond potential goes smoothly to a local maximum. If a bond length ever becomes > Rc, LAMMPS "breaks" the bond, which means two things. First, the bond potential is turned off by setting its type to 0, and is no longer computed. Second, a pairwise interaction between the two atoms is turned on, since they are no longer bonded.

LAMMPS does the second task via a computational sleight-of-hand. It subtracts the pairwise interaction as part of the bond computation. When the bond breaks, the subtraction stops. For this to work, the pairwise interaction must always be computed by the pair_style command, whether the bond is broken or not. This means that special_bonds must be set to 1,1,1, as indicated as a restriction below.
Note that when bonds are dumped to a file via the `dump local` command, bonds with type 0 are not included. The `delete_bonds` command can also be used to query the status of broken bonds or permanently delete them, e.g.:

```
delete_bonds all stats
delete_bonds all bond 0 remove
```

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**

This bond style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

The `quartic` style requires that `special_bonds` parameters be set to 1,1,1. Three- and four-body interactions (angle, dihedral, etc) cannot be used with `quartic` bonds.

**Related commands:**

`bond_coeff`, `delete_bonds`

**Default:** none
bond_style command

Syntax:

bond_style style args

- style = none or hybrid or class2 or fene or fene/expand or harmonic or morse or nonlinear or quartic

args = none for any style except hybrid
hybrid args = list of one or more styles

Examples:

bond_style harmonic
bond_style fene
bond_style hybrid harmonic fene

Description:

Set the formula(s) LAMMPS uses to compute bond interactions between pairs of atoms. In LAMMPS, a bond differs from a pairwise interaction, which are set via the pair_style command. Bonds are defined between specified pairs of atoms and remain in force for the duration of the simulation (unless the bond breaks which is possible in some bond potentials). The list of bonded atoms is read in by a read_data or read_restart command from a data or restart file. By contrast, pair potentials are typically defined between all pairs of atoms within a cutoff distance and the set of active interactions changes over time.

Hybrid models where bonds are computed using different bond potentials can be setup using the hybrid bond style.

The coefficients associated with a bond style can be specified in a data or restart file or via the bond_coeff command.

All bond potentials store their coefficient data in binary restart files which means bond_style and bond_coeff commands do not need to be re-specified in an input script that restarts a simulation. See the read_restart command for details on how to do this. The one exception is that bond_style hybrid only stores the list of sub-styles in the restart file; bond coefficients need to be re-specified.

IMPORTANT NOTE: When both a bond and pair style is defined, the special_bonds command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between 2 bonded atoms.

In the formulas listed for each bond style, \( r \) is the distance between the 2 atoms in the bond.

Here is an alphabetic list of bond styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated bond_coeff command.

Note that there are also additional bond styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the bond section of this page.

- bond_style none - turn off bonded interactions
- bond_style hybrid - define multiple styles of bond interactions
- `bond_style class2` - COMPASS (class 2) bond
- `bond_style fene` - FENE (finite-extensible non-linear elastic) bond
- `bond_style fene/expand` - FENE bonds with variable size particles
- `bond_style harmonic` - harmonic bond
- `bond_style morse` - Morse bond
- `bond_style nonlinear` - nonlinear bond
- `bond_style quartic` - breakable quartic bond
- `bond_style table` - tabulated by bond length

**Restrictions:**

Bond styles can only be set for atom styles that allow bonds to be defined.

Most bond styles are part of the MOLECULAR package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual bond potentials tell if it is part of a package.

**Related commands:**

`bond_coeff`, `delete_bonds`

**Default:**

`bond_style none`
bond_style table command

bond_style table/omp command

Syntax:

bond_style table style N

- style = linear or spline = method of interpolation
- N = use N values in table

Examples:

bond_style table linear 1000
bond_coeff 1 file.table ENTRY1

Description:

Style table creates interpolation tables of length N from bond potential and force values listed in a file(s) as a function of bond length. The files are read by the bond_coeff command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and force values at each of N distances. During a simulation, these tables are used to interpolate energy and force values as needed. The interpolation is done in one of 2 styles: linear or spline.

For the linear style, the bond length is used to find 2 surrounding table values from which an energy or force is computed by linear interpolation.

For the spline style, a cubic spline coefficients are computed and stored at each of the N values in the table. The bond length is used to find the appropriate set of coefficients which are used to evaluate a cubic polynomial which computes the energy or force.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above.

- filename
- keyword

The filename specifies a file containing tabulated energy and force values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# Bond potential for harmonic (one or more comment or blank lines)

HAM                           (keyword is the first text on line)
N 101 FP 0 0 EQ 0.5           (N, FP, EQ parameters)
  (blank line)
1 0.00 338.0000 1352.0000     (index, bond-length, energy, force)
2 0.01 324.6152 1324.9600
...                          
101 1.00 338.0000 -1352.0000
```
A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the bond_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the \(N\) specified in the bond_style table command. Let \(N_{\text{table}} = N\) in the bond_style command, and \(N_{\text{file}} = "N"\) in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the \(N_{\text{file}}\) tabulated values as nodal points. It uses these to interpolate as needed to generate energy and force values at \(N_{\text{table}}\) different points. The resulting tables of length \(N_{\text{table}}\) are then used as described above, when computing energy and force for individual bond lengths. This means that if you want the interpolation tables of length \(N_{\text{table}}\) to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set \(N_{\text{table}} = N_{\text{file}}\).

The "FP" parameter is optional. If used, it is followed by two values \(fplo\) and \(fphi\), which are the derivatives of the force at the innermost and outermost bond lengths. These values are needed by the spline construction routines. If not specified by the "FP" parameter, they are estimated (less accurately) by the first two and last two force values in the table.

The "EQ" parameter is also optional. If used, it is followed by a the equilibrium bond length, which is used, for example, by the fix shake command. If not used, the equilibrium bond length is set to 0.0.

Following a blank line, the next \(N\) lines list the tabulated values. On each line, the 1st value is the index from 1 to \(N\), the 2nd value is the bond length \(r\) (in distance units), the 3rd value is the energy (in energy units), and the 4th is the force (in force units). The bond lengths must range from a LO value to a HI value, and increase from one line to the next. If the actual bond length is ever smaller than the LO value or larger than the HI value, then the bond energy and force is evaluated as if the bond were the LO or HI length.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

**Restrictions:**

This bond style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

**Related commands:**
bond_coeff, delete_bonds

**Default:** none
boundary command

Syntax:

boundary x y z

• x,y,z = p or s or f or m, one or two letters

p is periodic
f is non-periodic and fixed
s is non-periodic and shrink-wrapped
m is non-periodic and shrink-wrapped with a minimum value

Examples:

boundary p p f
boundary p fs p
boundary s f fm

Description:

Set the style of boundaries for the global simulation box in each dimension. A single letter assigns the same style to both the lower and upper face of the box. Two letters assigns the first style to the lower face and the second style to the upper face. The initial size of the simulation box is set by the read_data, read_restart, or create_box commands.

The style p means the box is periodic, so that particles interact across the boundary, and they can exit one end of the box and re-enter the other end. A periodic dimension can change in size due to constant pressure boundary conditions or box deformation (see the fix npt and fix deform commands). The p style must be applied to both faces of a dimension.

The styles f, s, and m mean the box is non-periodic, so that particles do not interact across the boundary and do not move from one side of the box to the other. For style f, the position of the face is fixed. If an atom moves outside the face it may be lost. For style s, the position of the face is set so as to encompass the atoms in that dimension (shrink-wrapping), no matter how far they move. For style m, shrink-wrapping occurs, but is bounded by the value specified in the data or restart file or set by the create_box command. For example, if the upper z face has a value of 50.0 in the data file, the face will always be positioned at 50.0 or above, even if the maximum z-extent of all the atoms becomes less than 50.0.

For triclinic (non-orthogonal) simulation boxes, if the 2nd dimension of a tilt factor (e.g. y for xy) is periodic, then the periodicity is enforced with the tilt factor offset. If the 1st dimension is shrink-wrapped, then the shrink wrapping is applied to the tilted box face, to encompass the atoms. E.g. for a positive xy tilt, the xlo and xhi faces of the box are planes tilting in the +y direction as y increases. These tilted planes are shrink-wrapped around the atoms to determine the x extent of the box.

See Section_howto 12 of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

Restrictions:

This command cannot be used after the simulation box is defined by a read_data or create_box command or
read_restart command. See the change_box command for how to change the simulation box boundaries after it has been defined.

For 2d simulations, the z dimension must be periodic.

**Related commands:**

See the thermo_modify command for a discussion of lost atoms.

**Default:**

```
boundary p p p
```
box command

Syntax:

box keyword value ...

- one or more keyword/value pairs may be appended
- keyword = tilt

  \[\text{tilt value = small or large}\]

Examples:

box tilt large
box tilt small

Description:

Set attributes of the simulation box.

For triclinic (non-orthogonal) simulation boxes, the \textit{tilt} keyword allows simulation domains to be created with arbitrary tilt factors, e.g. via the \texttt{create_box} or \texttt{read_data} commands. Tilt factors determine how skewed the triclinic box is; see this section of the manual for a discussion of triclinic boxes in LAMMPS.

LAMMPS normally requires that no tilt factor can skew the box more than half the distance of the parallel box length, which is the 1st dimension in the tilt factor (x for xz). If \textit{tilt} is set to \texttt{small}, which is the default, then an error will be generated if a box is created which exceeds this limit. If \textit{tilt} is set to \texttt{large}, then no limit is enforced. You can create a box with any tilt factors you wish.

Note that if a simulation box has a large tilt factor, LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

Restrictions:

This command cannot be used after the simulation box is defined by a \texttt{read_data} or \texttt{create_box} command or \texttt{read_restart} command.

Related commands: none

Default:

The default value is tilt = small.
change_box command

Syntax:

change_box group-ID parameter args ... keyword args ...

- group-ID = ID of group of atoms to (optionally) displace
- one or more parameter/arg pairs may be appended

 parameter = x or y or z or xy or xz or yz or boundary or ortho or triclinic or set or remap
 x, y, z args = style value(s)
   style = final or delta or scale or volume
   final values = lo hi
     lo hi = box boundaries after displacement (distance units)
   delta values = dlo dhi
     dlo dhi = change in box boundaries after displacement (distance units)
   scale values = factor
     factor = multiplicative factor for change in box length after displacement
   volume value = none = adjust this dim to preserve volume of system
   xy, xz, yz args = style value
     style = final or delta
     final value = tilt
       tilt = tilt factor after displacement (distance units)
     delta value = dtilt
       dtilt = change in tilt factor after displacement (distance units)
 boundary args = x y z
   x, y, z = p or s or f or m, one or two letters
   p is periodic
   f is non-periodic and fixed
   s is non-periodic and shrink-wrapped
   m is non-periodic and shrink-wrapped with a minimum value
 ortho args = none = change box to orthogonal
 triclinic args = none = change box to triclinic
 set args = none = store state of current box
 remap args = none = remap atom coords from last saved state to current box

- zero or more keyword/value pairs may be appended
- keyword = units

 units value = lattice or box
 lattice = distances are defined in lattice units
 box = distances are defined in simulation box units

Examples:

change_box all xy final -2.0 z final 0.0 5.0 boundary p p f remap units box
change_box all x scale 1.1 y volume z volume remap

Description:

Change the volume and/or shape and/or boundary conditions for the simulation box. Orthogonal simulation boxes have 3 adjustable size parameters (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable size/shape parameters (x,y,z,xy,xz,yz). Any or all of them can be adjusted independently by this command. Thus it can be used to expand or contract a box, or to apply a shear strain to a non-orthogonal box. It can also be used to change the boundary conditions for the simulation box, similar to the boundary command.
The size and shape of the initial simulation box are specified by the create_box or read_data or read_restart command used to setup the simulation. The size and shape may be altered by subsequent runs, e.g. by use of the fix npt or fix deform commands. The create_box, read_data, and read_restart commands also determine whether the simulation box is orthogonal or triclinic and their doc pages explain the meaning of the xy,xz,yz tilt factors.

See Section_howto 12 of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

The keywords used in this command are applied sequentially to the simulation box and the atoms in it, in the order specified.

Before the sequence of keywords are invoked, the current box size/shape is stored, in case a remap keyword is used to map the atom coordinates from a previously stored box size/shape to the current one.

After all the keywords have been processed, any shrink-wrap boundary conditions are invoked (see the boundary command) which may change simulation box boundaries, and atoms are migrated to new owning processors.

IMPORTANT NOTE: Unlike the earlier "displace_box" version of this command, atom remapping is NOT performed by default. This command allows remapping to be done in a more general way, exactly when you specify it (zero or more times) in the sequence of transformations. Thus if you do not use the remap keyword, atom coordinates will not be changed even if the box size/shape changes. If a uniformly strained state is desired, the remap keyword should be specified.

IMPORTANT NOTE: It is possible to lose atoms with this command. E.g. by changing the box without remapping the atoms, and having atoms end up outside of non-periodic boundaries. It is also possible to alter bonds between atoms straddling a boundary in bad ways. E.g. by converting a boundary from periodic to non-periodic. It is also possible when remapping atoms to put them (nearly) on top of each other. E.g. by converting a boundary from non-periodic to periodic. All of these will typically lead to bad dynamics and/or generate error messages.

IMPORTANT NOTE: The simulation box size/shape can be changed by arbitrarily large amounts by this command. This is not a problem, except that the mapping of processors to the simulation box is not changed from its initial 3d configuration; see the processors command. Thus, if the box size/shape changes dramatically, the mapping of processors to the simulation box may not end up as optimal as the initial mapping attempted to be.

IMPORTANT NOTE: Because the keywords used in this command are applied one at a time to the simulation box and the atoms in it, care must be taken with triclinic cells to avoid exceeding the limits on skew after each transformation in the sequence. If skew is exceeded before the final transformation this can be avoided by changing the order of the sequence, or breaking the transformation into two or more smaller transformations. For more information on the allowed limits for box skew see the discussion on triclinic boxes on this page.

For the x, y, and z parameters, this is the meaning of their styles and values.

For style final, the final lo and hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style delta, plus or minus changes in the lo/hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style scale, a multiplicative factor to apply to the box length of a dimension is specified. For example, if the initial box length is 10, and the factor is 1.1, then the final box length will be 11. A factor less than 1.0 means compression.
The volume style changes the specified dimension in such a way that the overall box volume remains constant with respect to the operation performed by the preceding keyword. The volume style can only be used following a keyword that changed the volume, which is any of the x, y, z keywords. If the preceding keyword "key" had a volume style, then both it and the current keyword apply to the keyword preceding "key". I.e. this sequence of keywords is allowed:

change_box all x scale 1.1 y volume z volume

The volume style changes the associated dimension so that the overall box volume is unchanged relative to its value before the preceding keyword was invoked.

If the following command is used, then the z box length will shrink by the same 1.1 factor the x box length was increased by:

change_box all x scale 1.1 z volume

If the following command is used, then the y,z box lengths will each shrink by sqrt(1.1) to keep the volume constant. In this case, the y,z box lengths shrink so as to keep their relative aspect ratio constant:

change_box all"x scale 1.1 y volume z volume

If the following command is used, then the final box will be a factor of 10% larger in x and y, and a factor of 21% smaller in z, so as to keep the volume constant:

change_box all x scale 1.1 z volume y scale 1.1 z volume

IMPORTANT NOTE: For solids or liquids, when one dimension of the box is expanded, it may be physically undesirable to hold the other 2 box lengths constant since that implies a density change. For solids, adjusting the other dimensions via the volume style may make physical sense (just as for a liquid), but may not be correct for materials and potentials whose Poisson ratio is not 0.5.

For the scale and volume styles, the box length is expanded or compressed around its mid point.

For the xy, xz, and yz parameters, this is the meaning of their styles and values. Note that changing the tilt factors of a triclinic box does not change its volume.

For style final, the final tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

For style delta, a plus or minus change in the tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

All of these styles change the xy, xz, yz tilt factors. In LAMMPS, tilt factors (xy,xz,yz) for triclinic boxes are required to be no more than half the distance of the parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all equivalent. Any tilt factor specified by this command must be within these limits.

The boundary keyword takes arguments that have exactly the same meaning as they do for the boundary command. In each dimension, a single letter assigns the same style to both the lower and upper face of the box. Two letters assigns the first style to the lower face and the second style to the upper face.
The style $p$ means the box is periodic; the other styles mean non-periodic. For style $f$, the position of the face is fixed. For style $s$, the position of the face is set so as to encompass the atoms in that dimension (shrink-wrapping), no matter how far they move. For style $m$, shrink-wrapping occurs, but is bounded by the current box edge in that dimension, so that the box will become no smaller. See the boundary command for more explanation of these style options.

Note that the "boundary" command itself can only be used before the simulation box is defined via a read_data or create_box or read_restart command. This command allows the boundary conditions to be changed later in your input script. Also note that the read_restart will change boundary conditions to match what is stored in the restart file. So if you wish to change them, you should use the change_box command after the read_restart command.

The ortho and triclinic keywords convert the simulation box to be orthogonal or triclinic (non-orthogonal). See this section for a discussion of how non-orthogonal boxes are represented in LAMMPS.

The simulation box is defined as either orthogonal or triclinic when it is created via the create_box, read_data, or read_restart commands.

These keywords allow you to toggle the existing simulation box from orthogonal to triclinic and vice versa. For example, an initial equilibration simulation can be run in an orthogonal box, the box can be toggled to triclinic, and then a non-equilibrium MD (NEMD) simulation can be run with deformation via the fix deform command.

If the simulation box is currently triclinic and has non-zero tilt in xy, yz, or xz, then it cannot be converted to an orthogonal box.

The set keyword saves the current box size/shape. This can be useful if you wish to use the remap keyword more than once or if you wish it to be applied to an intermediate box size/shape in a sequence of keyword operations. Note that the box size/shape is saved before any of the keywords are processed, i.e. the box size/shape at the time the create_box command is encountered in the input script.

The remap keyword remaps atom coordinates from the last saved box size/shape to the current box state. For example, if you stretch the box in the x dimension or tilt it in the xy plane via the x and xy keywords, then the remap command will dilate or tilt the atoms to conform to the new box size/shape, as if the atoms moved with the box as it deformed.

Note that this operation is performed without regard to periodic boundaries. Also, any shrink-wrapping of non-periodic boundaries (see the boundary command) occurs after all keywords, including this one, have been processed.

Only atoms in the specified group are remapped.

The units keyword determines the meaning of the distance units used to define various arguments. A box value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A lattice value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing.

Restrictions:

If you use the ortho or triclinic keywords, then at the point in the input script when this command is issued, no dumps can be active, nor can a fix ave/spatial or fix deform be active. This is because these commands test whether the simulation box is orthogonal when they are first issued. Note that these commands can be used in your script before a change_box command is issued, so long as an undump or unfix command is also used to turn them off.
Related commands:

fix deform, boundary

Default:

The option default is units = lattice.
clear command

Syntax:

clear

Examples:

(commands for 1st simulation)
clear
(commands for 2nd simulation)

Description:

This command deletes all atoms, restores all settings to their default values, and frees all memory allocated by LAMMPS. Once a clear command has been executed, it is as if LAMMPS were starting over, with only the exceptions noted below. This command enables multiple jobs to be run sequentially from one input script.

These settings are not affected by a clear command: the working directory (shell command), log file status (log command), echo status (echo command), and input script variables (variable command).

Restrictions: none

Related commands: none

Default: none
communicate command

Syntax:

communicate style keyword value ...

- style = single or multi
- zero or more keyword/value pairs may be appended
- keyword = cutoff or group or vel

  cutoff value = Rcut (distance units) = communicate atoms from this far away
  group value = group-ID = only communicate atoms in the group
  vel value = yes or no = do or do not communicate velocity info with ghost atoms

Examples:

communicate multi
communicate multi group solvent
communicate single vel yes
communicate single cutoff 5.0 vel yes

Description:

This command sets the style of inter-processor communication that occurs each timestep as atom coordinates and other properties are exchanged between neighboring processors and stored as properties of ghost atoms.

The default style is single which means each processor acquires information for ghost atoms that are within a single distance from its sub-domain. The distance is the maximum of the neighbor cutoff for all atom type pairs.

For many systems this is an efficient algorithm, but for systems with widely varying cutoffs for different type pairs, the multi style can be faster. In this case, each atom type is assigned its own distance cutoff for communication purposes, and fewer atoms will be communicated. See the neighbor multi command for a neighbor list construction option that may also be beneficial for simulations of this kind.

The cutoff option allows you to set a ghost cutoff distance, which is the distance from the borders of a processor's sub-domain at which ghost atoms are acquired from other processors. By default the ghost cutoff = neighbor cutoff = pairwise force cutoff + neighbor skin. See the neighbor command for more information about the skin distance. If the specified Rcut is greater than the neighbor cutoff, then extra ghost atoms will be acquired. If it is smaller, the ghost cutoff is set to the neighbor cutoff.

These are simulation scenarios in which it may be useful to set a ghost cutoff > neighbor cutoff:

- a single polymer chain with bond interactions, but no pairwise interactions
- bonded interactions (e.g. dihedrals) extend further than the pairwise cutoff
- ghost atoms beyond the pairwise cutoff are needed for some computation

In the first scenario, a pairwise potential may not be defined. Thus the pairwise neighbor cutoff will be 0.0. But ghost atoms are still needed for computing bond, angle, etc interactions between atoms on different processors. The appropriate ghost cutoff depends on the newton bond setting. For newton bond off, the distance needs to be the furthest distance between any two atoms in the bond, angle, etc. E.g. the distance between 1-4 atoms in a dihedral. For newton bond on, the distance between the central atom in the bond, angle, etc and any other atom is...
sufficient. E.g. the distance between 2-4 atoms in a dihedral.

In the second scenario, a pairwise potential is defined, but its neighbor cutoff is not sufficiently long enough to enable bond, angle, etc terms to be computed. As in the previous scenario, an appropriate ghost cutoff should be set.

In the last scenario, a fix or compute or pairwise potential needs to calculate with ghost atoms beyond the normal pairwise cutoff for some computation it performs (e.g. locate neighbors of ghost atoms in a multibody pair potential). Setting the ghost cutoff appropriately can insure it will find the needed atoms.

The group option will limit communication to atoms in the specified group. This can be useful for models where no ghost atoms are needed for some kinds of particles. All atoms (not just those in the specified group) will still migrate to new processors as they move. The group specified with this option must also be specified via the atom_modify first command.

The vel option enables velocity information to be communicated with ghost particles. Depending on the atom_style, velocity info includes the translational velocity, angular velocity, and angular momentum of a particle. If the vel option is set to yes, then ghost atoms store these quantities; if no then they do not. The yes setting is needed by some pair styles which require the velocity state of both the I and J particles to compute a pairwise I,J interaction.

Note that if the fix deform command is being used with its "remap v" option enabled, then the velocities for ghost atoms (in the fix deform group) mirrored across a periodic boundary will also include components due to any velocity shift that occurs across that boundary (e.g. due to dilation or shear).

Restrictions: none

Related commands:

neighbor

Default:

The default settings are style = single, group = all, cutoff = 0.0, vel = no. The cutoff default of 0.0 means that ghost cutoff = neighbor cutoff = pairwise force cutoff + neighbor skin.
compute command

Syntax:

compute ID group-ID style args

- ID = user-assigned name for the computation
- group-ID = ID of the group of atoms to perform the computation on
- style = one of a list of possible style names (see below)
- args = arguments used by a particular style

Examples:

compute 1 all temp
compute newtemp flow temp/partial 1 1 0
compute 3 all ke/atom

Description:

Define a computation that will be performed on a group of atoms. Quantities calculated by a compute are instantaneous values, meaning they are calculated from information about atoms on the current timestep or iteration, though a compute may internally store some information about a previous state of the system. Defining a compute does not perform a computation. Instead computes are invoked by other LAMMPS commands as needed, e.g. to calculate a temperature needed for a thermostat fix or to generate thermodynamic or dump file output. See this howto section for a summary of various LAMMPS output options, many of which involve computes.

The ID of a compute can only contain alphanumeric characters and underscores.

Computes calculate one of three styles of quantities: global, per-atom, or local. A global quantity is one or more system-wide values, e.g. the temperature of the system. A per-atom quantity is one or more values per atom, e.g. the kinetic energy of each atom. Per-atom values are set to 0.0 for atoms not in the specified compute group. Local quantities are calculated by each processor based on the atoms it owns, but there may be zero or more per atom, e.g. a list of bond distances. Computes that produce per-atom quantities have the word "atom" in their style, e.g. ke/atom. Computes that produce local quantities have the word "local" in their style, e.g. bond/local. Styles with neither "atom" or "local" in their style produce global quantities.

Note that a single compute produces either global or per-atom or local quantities, but never more than one of these.

Global, per-atom, and local quantities each come in three kinds: a single scalar value, a vector of values, or a 2d array of values. The doc page for each compute describes the style and kind of values it produces, e.g. a per-atom vector. Some computes produce more than one kind of a single style, e.g. a global scalar and a global vector.

When a compute quantity is accessed, as in many of the output commands discussed below, it can be referenced via the following bracket notation, where ID is the ID of the compute:

<table>
<thead>
<tr>
<th>c_ID</th>
<th>entire scalar, vector, or array</th>
</tr>
</thead>
<tbody>
<tr>
<td>c_ID[I]</td>
<td>one element of vector, one column of array</td>
</tr>
<tr>
<td>c_ID[I][J]</td>
<td>one element of array</td>
</tr>
</tbody>
</table>
In other words, using one bracket reduces the dimension of the quantity once (vector -> scalar, array -> vector). Using two brackets reduces the dimension twice (array -> scalar). Thus a command that uses scalar compute values as input can also process elements of a vector or array.

Note that commands and variables which use compute quantities typically do not allow for all kinds, e.g. a command may require a vector of values, not a scalar. This means there is no ambiguity about referring to a compute quantity as c_ID even if it produces, for example, both a scalar and vector. The doc pages for various commands explain the details.

In LAMMPS, the values generated by a compute can be used in several ways:

- The results of computes that calculate a global temperature or pressure can be used by fixes that do thermostatting or barostatting or when atom velocities are created.
- Global values can be output via the thermo_style custom or fix ave/time command. Or the values can be referenced in a variable equal or variable atom command.
- Per-atom values can be output via the dump custom command or the fix ave/spatial command. Or they can be time-averaged via the fix ave/atom command or reduced by the compute reduce command. Or the per-atom values can be referenced in an atom-style variable.
- Local values can be reduced by the compute reduce command, or histogrammed by the fix ave/histo command, or output by the dump local command.

The results of computes that calculate global quantities can be either "intensive" or "extensive" values. Intensive means the value is independent of the number of atoms in the simulation, e.g. temperature. Extensive means the value scales with the number of atoms in the simulation, e.g. total rotational kinetic energy. Thermodynamic output will normalize extensive values by the number of atoms in the system, depending on the "thermo_modify norm" setting. It will not normalize intensive values. If a compute value is accessed in another way, e.g. by a variable, you may want to know whether it is an intensive or extensive value. See the doc page for individual computes for further info.

LAMMPS creates its own computes internally for thermodynamic output. Three computes are always created, named "thermo_temp", "thermo_press", and "thermo_pe", as if these commands had been invoked in the input script:

```plaintext
compute thermo_temp all temp
compute thermo_press all pressure thermo_temp
compute thermo_pe all pe
```

Additional computes for other quantities are created if the thermo style requires it. See the documentation for the thermo_style command.

Fixes that calculate temperature or pressure, i.e. for thermostatting or barostatting, may also create computes. These are discussed in the documentation for specific fix commands.

In all these cases, the default computes LAMMPS creates can be replaced by computes defined by the user in the input script, as described by the thermo_modify and fix modify commands.

Properties of either a default or user-defined compute can be modified via the compute_modify command.

Computes can be deleted with the uncompute command.

Code for new computes can be added to LAMMPS (see this section of the manual) and the results of their calculations accessed in the various ways described above.
Each compute style has its own doc page which describes its arguments and what it does. Here is an alphabetic list of compute styles available in LAMMPS:

- **angle/local** - theta and energy of each angle
- **atom/molecule** - sum per-atom properties for each molecule
- **bond/local** - distance and energy of each bond
- **centro/atom** - centro-symmetry parameter for each atom
- **cluster/atom** - cluster ID for each atom
- **cna/atom** - common neighbor analysis (CNA) for each atom
- **com** - center-of-mass of group of atoms
- **com/molecule** - center-of-mass for each molecule
- **contact/atom** - contact count for each spherical particle
- **coord/atom** - coordination number for each atom
- **damage/atom** - Peridynamic damage for each atom
- **dihedral/local** - angle of each dihedral
- **displace/atom** - displacement of each atom
- **erotate/asphere** - rotational energy of aspherical particles
- **erotate/sphere** - rotational energy of spherical particles
- **erotate/sphere/atom** - rotational energy for each spherical particle
- **event/displace** - detect event on atom displacement
- **group/group** - energy/force between two groups of atoms
- **gyration** - radius of gyration of group of atoms
- **gyration/molecule** - radius of gyration for each molecule
- **heat/flux** - heat flux through a group of atoms
- **improper/local** - angle of each improper
- **ke** - translational kinetic energy
- **ke/atom** - kinetic energy for each atom
- **msd** - mean-squared displacement of group of atoms
- **msd/molecule** - mean-squared displacement for each molecule
- **pair** - values computed by a pair style
- **pair/local** - distance/energy/force of each pairwise interaction
- **pe** - potential energy
- **pe/atom** - potential energy for each atom
- **pressure** - total pressure and pressure tensor
- **property/atom** - convert atom attributes to per-atom vectors/arrays
- **property/local** - convert local attributes to localvectors/arrays
- **property/molecule** - convert molecule attributes to localvectors/arrays
- **rdf** - radial distribution function g(r) histogram of group of atoms
- **reduce** - combine per-atom quantities into a single global value
- **reduce/region** - same as compute reduce, within a region
- **slice** - extract values from global vector or array
- **stress/atom** - stress tensor for each atom
- **temp** - temperature of group of atoms
- **temp/asphere** - temperature of aspherical particles
- **temp/com** - temperature after subtracting center-of-mass velocity
- **temp/deform** - temperature excluding box deformation velocity
- **temp/partial** - temperature excluding one or more dimensions of velocity
- **temp/profile** - temperature excluding a binned velocity profile
- **temp/ramp** - temperature excluding ramped velocity component
- **temp/region** - temperature of a region of atoms
- **temp/sphere** - temperature of spherical particles
• ti - thermodynamic integration free energy values

There are also additional compute styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the compute section of this page.

There are also additional accelerated compute styles included in the LAMMPS distribution for faster performance on CPUs and GPUs. The list of these with links to the individual styles are given in the pair section of this page.

Restrictions: none

Related commands:
uncompute, compute_modify, fix ave/atom, fix ave/spatial, fix ave/time, fix ave/histo

Default: none
compute ackland/atom command

Syntax:

compute ID group-ID ackland/atom

• ID, group-ID are documented in compute command
• ackland/atom = style name of this compute command

Examples:

compute 1 all ackland/atom

Description:

Defines a computation that calculates the local lattice structure according to the formulation given in (Ackland).

In contrast to the centro-symmetry parameter this method is stable against temperature boost, because it is based not on the distance between particles but the angles. Therefore statistical fluctuations are averaged out a little more. A comparison with the Common Neighbor Analysis metric is made in the paper.

The result is a number which is mapped to the following different lattice structures:

• 0 = UNKNOWN
• 1 = BCC
• 2 = FCC
• 3 = HCP
• 4 = ICO

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each of which computes this quantity.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section howto 15 for an overview of LAMMPS output options.

Restrictions:

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The per-atom vector values will be unitless since they are the integers defined above.

Related commands:

compute centro/atom

Default: none
**compute angle/local command**

Syntax:

```
compute ID group-ID angle/local input1 input2 ...
```

- ID, group-ID are documented in [compute command](#)
- angle/local = style name of this compute command
- zero or more keywords may be appended
- keyword = *theta* or *eng*

  *theta* = tabulate angles
  *eng* = tabulate angle energies

**Examples:**

```
compute 1 all angle/local theta
compute 1 all angle/local eng theta
```

**Description:**

Define a computation that calculates properties of individual angle interactions. The number of datums generated, aggregated across all processors, equals the number of angles in the system.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their angles. An angle will only be included if all 3 atoms in the angle are in the specified compute group. Any angles that have been broken (see the [angle_style command](#)) by setting their angle type to 0 are not included. Angles that have been turned off (see the [fix shake](#) or [delete_bonds](#) commands) by setting their angle type negative are written into the file, but their energy will be 0.0.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, angle output from the [compute property/local](#) command can be combined with data from this command and output by the [dump local](#) command in a consistent way.

**Output info:**

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of angles. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See [this section](#) for an overview of LAMMPS output options.

The output for *theta* will be in degrees. The output for *eng* will be in energy units.

**Restrictions:** none

**Related commands:**

[dump local](#), [compute property/local](#)
Default: none
compute atom/molecule command

Syntax:
compute ID group-ID atom/molecule input1 input2 ...

- ID, group-ID are documented in compute command
- atom/molecule = style name of this compute command
- one or more inputs can be listed
- input = c_ID, c_ID[N], f_ID, f_ID[N], v_name

  c_ID = per-atom vector calculated by a compute with ID
  c_ID[I] = Ith column of per-atom array calculated by a compute with ID
  f_ID = per-atom vector calculated by a fix with ID
  f_ID[I] = Ith column of per-atom array calculated by a fix with ID
  v_name = per-atom vector calculated by an atom-style variable with name

Examples:
compute 1 all atom/molecule c_ke c_pe
compute 1 top atom/molecule v_myFormula c_stress

Description:

Define a calculation that sums per-atom values on a per-molecule basis, one per listed input. The inputs can
computes, fixes, or variables that generate per-atom quantities. Note that attributes stored by atoms, such as mass
or force, can also be summed on a per-molecule basis, by accessing these quantities via the compute
property/atom command.

Each listed input is operated on independently. Only atoms within the specified group contribute to the
per-molecule sum. Note that compute or fix inputs define their own group which may affect the quantities they
return. For example, if a compute is used as an input which generates a per-atom vector, it will generate values of
0.0 for atoms that are not in the group specified for that compute.

The ordering of per-molecule quantities produced by this compute is consistent with the ordering produced by
other compute commands that generate per-molecule datums. Conceptually, their molecule IDs will be in
ascending order for any molecule with one or more of its atoms in the specified group.

If an input begins with "c_", a compute ID must follow which has been previously defined in the input script and
which generates per-atom quantities. See the individual compute doc page for details. If no bracketed integer is
appended, the vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the
array calculated by the compute is used. Users can also write code for their own compute styles and add them to
LAMMPS.

If an input begins with "f_", a fix ID must follow which has been previously defined in the input script and which
generates per-atom quantities. See the individual fix doc page for details. Note that some fixes only produce their
values on certain timesteps, which must be compatible with when compute atom/molecule references the values,
else an error results. If no bracketed integer is appended, the vector calculated by the fix is used. If a bracketed
integer is appended, the Ith column of the array calculated by the fix is used. Users can also write code for their
own fix style and add them to LAMMPS.
If an input begins with "v_", a variable name must follow which has been previously defined in the input script. It must be an atom-style variable. Atom-style variables can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to sum on a per-molecule basis.

**Output info:**

This compute calculates a global vector or global array depending on the number of input values. The length of the vector or number of rows in the array is the number of molecules. If a single input is specified, a global vector is produced. If two or more inputs are specified, a global array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses global values from a compute as input. See this section for an overview of LAMMPS output options.

All the vector or array values calculated by this compute are "extensive".

The vector or array values will be in whatever units the input quantities are in.

**Restrictions:** none

**Related commands:**

compute, fix, variable

**Default:** none
compute bond/local command

Syntax:

compute ID group-ID bond/local input1 input2 ...

- ID, group-ID are documented in compute command
- bond/local = style name of this compute command
- zero or more keywords may be appended
- keyword = dist or eng

  dist = tabulate bond distances
  eng = tabulate bond energies

Examples:

compute 1 all bond/local eng
compute 1 all bond/local dist eng

Description:

Define a computation that calculates properties of individual bond interactions. The number of datums generated, aggregated across all processors, equals the number of bonds in the system.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their bonds. A bond will only be included if both atoms in the bond are in the specified compute group. Any bonds that have been broken (see the bond_style command) by setting their bond type to 0 are not included. Bonds that have been turned off (see the fix shake or delete_bonds commands) by setting their bond type negative are written into the file, but their energy will be 0.0.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, bond output from the compute property/local command can be combined with data from this command and output by the dump local command in a consistent way.

Here is an example of how to do this:

compute 1 all property/local batom1 batom2 btype
compute 2 all bond/local dist eng
dump 1 all local 1000 tmp.dump index c_11 c_12 c_13 c_21 c_22

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of bonds. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The output for dist will be in distance units. The output for eng will be in energy units.
Restrictions: none

Related commands:
dump local, compute property/local

Default: none
compute centro/atom command

Syntax:

compute ID group-ID centro/atom lattice

- ID, group-ID are documented in compute command
- centro/atom = style name of this compute command
- lattice = fcc or bcc or N = # of neighbors per atom to include

Examples:

compute 1 all centro/atom fcc
compute 1 all centro/atom 8

Description:

Define a computation that calculates the centro-symmetry parameter for each atom in the group. In solid-state systems the centro-symmetry parameter is a useful measure of the local lattice disorder around an atom and can be used to characterize whether the atom is part of a perfect lattice, a local defect (e.g. a dislocation or stacking fault), or at a surface.

The value of the centro-symmetry parameter will be 0.0 for atoms not in the specified compute group.

This parameter is computed using the following formula from (Kelchner)

\[ CS = \sum_{i=1}^{N/2} |\vec{R}_i + \vec{R}_{i+N/2}|^2 \]

where the \( N \) nearest neighbors or each atom are identified and \( \vec{R}_i \) and \( \vec{R}_{i+N/2} \) are vectors from the central atom to a particular pair of nearest neighbors. There are \( N(N-1)/2 \) possible neighbor pairs that can contribute to this formula. The quantity in the sum is computed for each, and the \( N/2 \) smallest are used. This will typically be for pairs of atoms in symmetrically opposite positions with respect to the central atom; hence the \( i+N/2 \) notation.

\( N \) is an input parameter, which should be set to correspond to the number of nearest neighbors in the underlying lattice of atoms. If the keyword \( fcc \) or \( bcc \) is used, \( N \) is set to 12 and 8 respectively. More generally, \( N \) can be set to a positive, even integer.

For an atom on a lattice site, surrounded by atoms on a perfect lattice, the centro-symmetry parameter will be 0. It will be near 0 for small thermal perturbations of a perfect lattice. If a point defect exists, the symmetry is broken, and the parameter will be a larger positive value. An atom at a surface will have a large positive parameter. If the atom does not have \( N \) neighbors (within the potential cutoff), then its centro-symmetry parameter is set to 0.0.

Only atoms within the cutoff of the pairwise neighbor list are considered as possible neighbors. Atoms not in the compute group are included in the \( N \) neighbors used in this calculation.
The neighbor list needed to compute this quantity is constructed each time the calculation is performed (e.g. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each with a centro/atom style.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section howto 15 for an overview of LAMMPS output options.

The per-atom vector values are unitless values >= 0.0. Their magnitude depends on the lattice style due to the number of contributing neighbor pairs in the summation in the formula above. And it depends on the local defects surrounding the central atom, as described above.

Here are typical centro-symmetry values, from a nanoindentation simulation into gold (FCC). These were provided by Jon Zimmerman (Sandia):

Bulk lattice = 0
Dislocation core ~ 1.0 (0.5 to 1.25)
Stacking faults ~ 5.0 (4.0 to 6.0)
Free surface ~ 23.0

These values are *not* normalized by the square of the lattice parameter. If they were, normalized values would be:

Bulk lattice = 0
Dislocation core ~ 0.06 (0.03 to 0.075)
Stacking faults ~ 0.3 (0.24 to 0.36)
Free surface ~ 1.38

For BCC materials, the values for dislocation cores and free surfaces would be somewhat different, due to their being only 8 neighbors instead of 12.

Restrictions: none

Related commands:

compute cna/atom

Default: none

compute cluster/atom command

Syntax:

compute ID group-ID cluster/atom cutoff

- ID, group-ID are documented in compute command
- cluster/atom = style name of this compute command
- cutoff = distance within which to label atoms as part of same cluster (distance units)

Examples:

compute 1 all cluster/atom 1.0

Description:

Define a computation that assigns each atom a cluster ID.

A cluster is defined as a set of atoms, each of which is within the cutoff distance from one or more other atoms in the cluster. If an atom has no neighbors within the cutoff distance, then it is a 1-atom cluster. The ID of every atom in the cluster will be the smallest atom ID of any atom in the cluster.

Only atoms in the compute group are clustered and assigned cluster IDs. Atoms not in the compute group are assigned a cluster ID = 0.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each of a cluster/atom style.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be an ID > 0, as explained above.

Restrictions: none

Related commands:

compute coord/atom

Default: none
compute cna/atom command

Syntax:

compute ID group-ID cna/atom cutoff

- ID, group-ID are documented in compute command
- cna/atom = style name of this compute command
- cutoff = cutoff distance for nearest neighbors (distance units)

Examples:

compute 1 all cna/atom 3.08

Description:

Define a computation that calculates the CNA (Common Neighbor Analysis) pattern for each atom in the group. In solid-state systems the CNA pattern is a useful measure of the local crystal structure around an atom. The CNA methodology is described in (Faken) and (Tsuzuki).

Currently, there are five kinds of CNA patterns LAMMPS recognizes:

- fcc = 1
- hcp = 2
- bcc = 3
- icosohedral = 4
- unknown = 5

The value of the CNA pattern will be 0 for atoms not in the specified compute group. Note that normally a CNA calculation should only be performed on mono-component systems.

The CNA calculation can be sensitive to the specified cutoff value. You should insure the appropriate nearest neighbors of an atom are found within the cutoff distance for the presumed crystal structure. E.g. 12 nearest neighbors for perfect FCC and HCP crystals, 14 nearest neighbors for perfect BCC crystals. These formulas can be used to obtain a good cutoff distance:

\[ r_{c}^{fcc} = \frac{1}{2} \left( \frac{\sqrt{2}}{2} + 1 \right) a \approx 0.8536 \ a \]

\[ r_{c}^{bcc} = \frac{1}{2} (\sqrt{2} + 1) a \approx 1.207 \ a \]

\[ r_{c}^{hcp} = \frac{1}{2} \left( 1 + \sqrt{\frac{4 + 2x^2}{3}} \right) a \]
where \( a \) is the lattice constant for the crystal structure concerned and in the HCP case, \( x = (c/a) / 1.633 \), where 1.633 is the ideal \( c/a \) for HCP crystals.

Also note that since the CNA calculation in LAMMPS uses the neighbors of an owned atom to find the nearest neighbors of a ghost atom, the following relation should also be satisfied:

\[
R_c + R_s > 2 \times \text{cutoff}
\]

where \( R_c \) is the cutoff distance of the potential, \( R_s \) is the skin distance as specified by the \texttt{neighbor} command, and \texttt{cutoff} is the argument used with the compute \texttt{cna/atom} command. LAMMPS will issue a warning if this is not the case.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (e.g. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each with a \texttt{cna/atom} style.

\textbf{Output info:}

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section\_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be a number from 0 to 5, as explained above.

\textbf{Restrictions:} none

\textbf{Related commands:}

\texttt{compute centro/atom}

\textbf{Default:} none


compute com command

Syntax:

compute ID group-ID com

• ID, group-ID are documented in compute command
• com = style name of this compute command

Examples:

compute 1 all com

Description:

Define a computation that calculates the center-of-mass of the group of atoms, including all effects due to atoms passing thru periodic boundaries.

A vector of three quantites is calculated by this compute, which are the x,y,z coordinates of the center of mass.

IMPORTANT NOTE: The coordinates of an atom contribute to the center-of-mass in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

IMPORTANT NOTE: If an atom is part of a rigid body (see the fix rigid command), it's periodic image flags are altered, and its contribution to the center-of-mass may not reflect its true contribution. See the fix rigid command for details. Thus, to compute the center-of-mass of rigid bodies as they cross periodic boundaries, you will need to post-process a dump file containing coordinates of the atoms in the bodies.

Output info:

This compute calculates a global vector of length 3, which can be accessed by indices 1-3 by any command that uses global vector values from a compute as input. See this section for an overview of LAMMPS output options.

The vector values are "intensive". The vector values will be in distance units.

Restrictions: none

Related commands:

compute com/molecule

Default: none
compute com/molecule command

Syntax:

compute ID group-ID com/molecule

- ID, group-ID are documented in compute command
- com/molecule = style name of this compute command

Examples:

compute 1 fluid com/molecule

Description:

Define a computation that calculates the center-of-mass of individual molecules. The calculation includes all effects due to atoms passing thru periodic boundaries.

The x,y,z coordinates of the center-of-mass for a particular molecule are only computed if one or more of its atoms are in the specified group. Normally all atoms in the molecule should be in the group, however this is not required. LAMMPS will warn you if this is not the case. Only atoms in the group contribute to the center-of-mass calculation for the molecule.

The ordering of per-molecule quantities produced by this compute is consistent with the ordering produced by other compute commands that generate per-molecule datums. Conceptually, them molecule IDs will be in ascending order for any molecule with one or more of its atoms in the specified group.

IMPORTANT NOTE: The coordinates of an atom contribute to the molecule's center-of-mass in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

IMPORTANT NOTE: If an atom is part of a rigid body (see the fix rigid command), it's periodic image flags are altered, and its contribution to the center-of-mass may not reflect its true contribution. See the fix rigid command for details. Thus, to compute the center-of-mass of rigid bodies as they cross periodic boundaries, you will need to post-process a dump file containing coordinates of the atoms in the bodies.

Output info:

This compute calculates a global array where the number of rows = Nmolecules and the number of columns = 3 for the x,y,z center-of-mass coordinates of each molecule. These values can be accessed by any command that uses global array values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in distance units.

Restrictions: none

Related commands:
compute com

**Default:** none
**compute contact/atom command**

**Syntax:**

`compute ID group-ID contact/atom`

- ID, group-ID are documented in compute command
- contact/atom = style name of this compute command

**Examples:**

`compute 1 all contact/atom`

**Description:**

Define a computation that calculates the number of contacts for each atom in a group.

The contact number is defined for finite-size spherical particles as the number of neighbor atoms which overlap the central particle, meaning that their distance of separation is less than or equal to the sum of the radii of the two particles.

The value of the contact number will be 0.0 for atoms not in the specified compute group.

**Output info:**

This compute calculates a per-atom vector, whose values can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be a number $\geq 0.0$, as explained above.

**Restrictions:**

This compute requires that atoms store a radius as defined by the atom_style sphere command.

**Related commands:**

`compute coord/atom`

**Default:** none
compute coord/atom command

Syntax:

compute ID group-ID coord/atom cutoff type1 type2 ...

- ID, group-ID are documented in compute command
- coord/atom = style name of this compute command
- cutoff = distance within which to count coordination neighbors (distance units)
- typeN = atom type for Nth coordination count (see asterisk form below)

Examples:

compute 1 all coord/atom 2.0
compute 1 all coord/atom 6.0 1 2
compute 1 all coord/atom 6.0 2*4 5*8 *

Description:

Define a computation that calculates one or more coordination numbers for each atom in a group.

A coordination number is defined as the number of neighbor atoms with specified atom type(s) that are within the specified cutoff distance from the central atom. Atoms not in the group are included in a coordination number of atoms in the group.

The typeN keywords allow you to specify which atom types contribute to each coordination number. One coordination number is computed for each of the typeN keywords listed. If no typeN keywords are listed, a single coordination number is calculated, which includes atoms of all types (same as the "*" format, see below).

The typeN keywords can be specified in one of two ways. An explicit numeric value can be used, as in the 2nd example above. Or a wild-card asterisk can be used to specify a range of atom types. This takes the form "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

The value of all coordination numbers will be 0.0 for atoms not in the specified compute group.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently.

Output info:

If single type1 keyword is specified (or if none are specified), this compute calculates a per-atom vector. If multiple typeN keywords are specified, this compute calculates a per-atom array, with N columns. These values can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector or array values will be a number >= 0.0, as explained above.

Restrictions: none
Related commands:

compute cluster/atom

Default: none
compute damage/atom command

Syntax:

compute ID group-ID damage/atom

- ID, group-ID are documented in compute command
- damage/atom = style name of this compute command

Examples:

compute 1 all damage/atom

Description:

Define a computation that calculates the per-atom damage for each atom in a group. Please see the PDLAMMPS user guide for a formal definition of "damage" and more details about Peridynamics as it is implemented in LAMMPS.

The value of the damage will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be a number >= 0.0, as explained above.

Restrictions:

This compute is part of the PERI package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

dump custom

Default: none
compute dihedral/local command

Syntax:

compute ID group-ID dihedral/local input1 input2 ...

- ID, group-ID are documented in compute command
- dihedral/local = style name of this compute command
- zero or more keywords may be appended
- keyword = phi

phi = tabulate dihedral angles

Examples:

compute 1 all dihedral/local phi

Description:

Define a computation that calculates properties of individual dihedral interactions. The number of datums generated, aggregated across all processors, equals the number of angles in the system.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their dihedrals. A dihedral will only be included if all 4 atoms in the dihedral are in the specified compute group.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, dihedral output from the compute property/local command can be combined with data from this command and output by the dump local command in a consistent way.

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of dihedrals. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The output for phi will be in degrees.

Restrictions: none

Related commands:

dump local, compute property/local

Default: none
compute displace/atom command

Syntax:

compute ID group-ID displace/atom

- ID, group-ID are documented in compute command
- displace/atom = style name of this compute command

Examples:

compute 1 all displace/atom

Description:

Define a computation that calculates the current displacement of each atom in the group from its original coordinates, including all effects due to atoms passing thru periodic boundaries.

A vector of four quantities per atom is calculated by this compute. The first 3 elements of the vector are the dx,dy,dz displacements. The 4th component is the total displacement, i.e. sqrt(dx*dx + dy*dy + dz*dz).

The displacement of an atom is from its original position at the time the compute command was issued. To store the original coordinates, the compute creates its own fix of style "store/state", as if this command had been issued:

fix compute-ID_store_state group-ID store/state xu yu zu

See the fix store/state command for details. Note that the ID of the new fix is the compute-ID + underscore + "store/state", and the group for the new fix is the same as the compute group.

The value of the displacement will be 0.0 for atoms not in the specified compute group.

IMPORTANT NOTE: Fix store/state stores the initial coordinates in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

IMPORTANT NOTE: If an atom is part of a rigid body (see the fix rigid command), it's periodic image flags are altered, and the computed displacement may not reflect its true displacement. See the fix rigid command for details. Thus, to compute the displacement of rigid bodies as they cross periodic boundaries, you will need to post-process a dump file containing coordinates of the atoms in the bodies.

IMPORTANT NOTE: If you want the quantities calculated by this compute to be continuous when running from a restart file, then you should use the same ID for this compute, as in the original run. This is so that the created fix will also have the same ID, and thus be initialized correctly with atom coordinates from the restart file.

Output info:

This compute calculates a per-atom array with 4 columns, which can be accessed by indices 1-4 by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.
The per-atom array values will be in distance units.

**Restrictions:** none

**Related commands:**
compute msd, dump custom, fix store/state

**Default:** none
compute erotate/asphere command

Syntax:

compute ID group-ID erotate/asphere

- ID, group-ID are documented in compute command
- erotate/asphere = style name of this compute command

Examples:

compute 1 all erotate/asphere

Description:

Define a computation that calculates the rotational kinetic energy of a group of aspherical particles. The aspherical particles can be ellipsoids, or line segments, or triangles. See the atom_style and read_data commands for descriptions of these options.

For all 3 types of particles, the rotational kinetic energy is computed as 1/2 I w^2, where I is the inertia tensor for the aspherical particle and w is its angular velocity, which is computed from its angular momentum if needed.

IMPORTANT NOTE: For 2d models, ellipsoidal particles are treated as ellipsoids, not ellipses, meaning their moments of inertia will be the same as in 3d.

Output info:

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions:

This compute requires that ellipsoidal particles atoms store a shape and quaternion orientation and angular momentum as defined by the atom_style ellipsoid command.

This compute requires that line segment particles atoms store a length and orientation and angular velocity as defined by the atom_style line command.

This compute requires that triangular particles atoms store a size and shape and quaternion orientation and angular momentum as defined by the atom_style tri command.

All particles in the group must be finite-size. They cannot be point particles.

Related commands: none

compute erotate/sphere

Default: none
compute erotate/sphere command

Syntax:

compute ID group-ID erotate/sphere

- ID, group-ID are documented in compute command
- erotate/sphere = style name of this compute command

Examples:

compute 1 all erotate/sphere

Description:

Define a computation that calculates the rotational kinetic energy of a group of spherical particles.

The rotational energy is computed as \( \frac{1}{2} I \omega^2 \), where \( I \) is the moment of inertia for a sphere and \( \omega \) is the particle's angular velocity.

IMPORTANT NOTE: For 2d models, particles are treated as spheres, not disks, meaning their moment of inertia will be the same as in 3d.

Output info:

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions:

This compute requires that atoms store a radius and angular velocity (omega) as defined by the atom_style sphere command.

All particles in the group must be finite-size spheres or point particles. They cannot be aspherical. Point particles will not contribute to the rotational energy.

Related commands:

compute erotate/asphere

Default: none
compute erotate/sphere/atom command

Syntax:

```
compute ID group-ID erotate/sphere/atom
```

- ID, group-ID are documented in `compute` command
- `erotate/sphere/atom` = style name of this compute command

Examples:

```
compute 1 all erotate/sphere/atom
```

Description:

Define a computation that calculates the rotational kinetic energy for each particle in a group.

The rotational energy is computed as \( \frac{1}{2} I w^2 \), where \( I \) is the moment of inertia for a sphere and \( w \) is the particle's angular velocity.

IMPORTANT NOTE: For 2d models, particles are treated as spheres, not disks, meaning their moment of inertia will be the same as in 3d.

The value of the rotational kinetic energy will be 0.0 for atoms not in the specified compute group or for point particles with a radius = 0.0.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions: none

Related commands:

dump custom

Default: none
compute event/displace command

Syntax:

compute ID group-ID event/displace threshold

- ID, group-ID are documented in compute command
- event/displace = style name of this compute command
- threshold = minimum distance any particle must move to trigger an event (distance units)

Examples:

compute 1 all event/displace 0.5

Description:

Define a computation that flags an "event" if any particle in the group has moved a distance greater than the specified threshold distance when compared to a previously stored reference state (i.e. the previous event). This compute is typically used in conjunction with the prd and tad commands, to detect if a transition to a new minimum energy basin has occurred.

This value calculated by the compute is equal to 0 if no particle has moved far enough, and equal to 1 if one or more particles have moved further than the threshold distance.

NOTE: If the system is undergoing significant center-of-mass motion, due to thermal motion, an external force, or an initial net momentum, then this compute will not be able to distinguish that motion from local atom displacements and may generate "false postives."

Output info:

This compute calculates a global scalar (the flag). This value can be used by any command that uses a global scalar value from a compute as input. See SectionHowto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The scalar value will be a 0 or 1 as explained above.

Restrictions:

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

Related commands:

prd, tad

Default: none
compute group/group command

Syntax:

compute ID group-ID group/group group2-ID keyword value ...

• ID, group-ID are documented in compute command
• group/group = style name of this compute command
• group2-ID = group ID of second (or same) group
• zero or more keyword/value pairs may be appended
• keyword = pair or kspace or boundary

pair value = yes or no
kspace value = yes or no
boundary value = yes or no

Examples:

compute 1 lower group/group upper
compute 1 lower group/group upper kspace yes
compute mine fluid group/group wall

Description:

Define a computation that calculates the total energy and force interaction between two groups of atoms: the compute group and the specified group2. The two groups can be the same.

If the pair keyword is set to yes, which is the default, then the interaction energy will include a pair component which is defined as the pairwise energy between all pairs of atoms where one atom in the pair is in the first group and the other is in the second group. Likewise, the interaction force calculated by this compute will include the force on the compute group atoms due to pairwise interactions with atoms in the specified group2.

If the kspace keyword is set to yes, which is not the default, and if a kspace_style is defined, then the interaction energy will include a Kspace component which is the long-range Coulombic energy between all the atoms in the first group and all the atoms in the 2nd group. Likewise, the interaction force calculated by this compute will include the force on the compute group atoms due to long-range Coulombic interactions with atoms in the specified group2.

Normally the long-range Coulombic energy converges only when the net charge of the unit cell is zero. However, one can assume the net charge of the system is neutralized by a uniform background plasma, and a correction to the system energy can be applied to reduce artifacts. For more information see (Bogusz). If the boundary keyword is set to yes, which is the default, and kspace contributions are included, then this energy correction term will be added to the total group-group energy. This correction term does not affect the force calculation and will be zero if one or both of the groups are charge neutral. This energy correction term is the same as that included in the regular Ewald and PPPM routines.

This compute does not calculate any bond or angle or dihedral or improper interactions between atoms in the two groups.

The pairwise contributions to the group-group interactions are calculated by looping over a neighbor list. The Kspace contribution to the group-group interactions require essentially the same amount of work (FFTs, Ewald
summation) as computing long-range forces for the entire system. Thus it can be costly to invoke this compute too
frequently.

If you desire a breakdown of the interactions into a pairwise and Kspace component, simply invoke the compute
twice with the appropriate yes/no settings for the pair and kspace keywords. This is no more costly than using a
single compute with both keywords set to yes. The individual contributions can be summed in a variable if
desired.

This document describes how the long-range group-group calculations are performed.

Output info:

This compute calculates a global scalar (the energy) and a global vector of length 3 (force), which can be accessed
by indices 1-3. These values can be used by any command that uses global scalar or vector values from a compute
as input. See this section for an overview of LAMMPS output options.

Both the scalar and vector values calculated by this compute are "extensive". The scalar value will be in energy
units. The vector values will be in force units.

Restrictions:

Not all pair styles can be evaluated in a pairwise mode as required by this compute. For example, 3-body and
other many-body potentials, such as Tersoff and Stillinger-Weber cannot be used. EAM potentials only include
the pair potential portion of the EAM interaction when used by this compute, not the embedding term.

Not all Kspace styles support calculation of group/group interactions. The ewald and pppm styles do.

Related commands: none

Default:

The option defaults are pair = yes, kspace = no, and boundary = yes.

compute gyration command

Syntax:

compute ID group-ID gyration

- ID, group-ID are documented in compute command
- gyration = style name of this compute command

Examples:

compute 1 molecule gyration

Description:

Define a computation that calculates the radius of gyration $R_g$ of the group of atoms, including all effects due to atoms passing thru periodic boundaries.

$R_g$ is a measure of the size of the group of atoms, and is computed by this formula

$$R_g^2 = \frac{1}{M} \sum_i m_i (r_i - r_{cm})^2$$

where $M$ is the total mass of the group, $r_{cm}$ is the center-of-mass position of the group, and the sum is over all atoms in the group.

A $R_g$ tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formula, except that $(r_i - r_{cm})^2$ is replaced by $(r_{ix} - r_{cmx}) (r_{iy} - r_{cmy})$ for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

IMPORTANT NOTE: The coordinates of an atom contribute to $R_g$ in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

Output info:

This compute calculates a global scalar ($R_g$) and a global vector of length 6 ($R_g$ tensor), which can be accessed by indices 1-6. These values can be used by any command that uses a global scalar value or vector values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar and vector values calculated by this compute are "intensive". The scalar and vector values will be in distance units.

Restrictions: none

Related commands:
compute gyration/molecule

Default: none
compute gyration/molecule command

Syntax:

compute ID group-ID gyration/molecule keyword value ...

- ID, group-ID are documented in compute command
- gyration/molecule = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = tensor

  tensor value = none

Examples:

compute 1 molecule gyration/molecule
compute 2 molecule gyration/molecule tensor

Description:

Define a computation that calculates the radius of gyration \( R_g \) of individual molecules. The calculation includes all effects due to atoms passing thru periodic boundaries.

\( R_g \) is a measure of the size of a molecule, and is computed by this formula

\[
R_g^2 = \frac{1}{M} \sum_i m_i (r_i - r_{cm})^2
\]

where \( M \) is the total mass of the molecule, \( r_{cm} \) is the center-of-mass position of the molecule, and the sum is over all atoms in the molecule and in the group.

If the tensor keyword is specified, then the scalar \( R_g \) value is not calculated, but an \( R_g \) tensor is instead calculated for each molecule. The formula for the components of the tensor is the same as the above formula, except that \((r_i - r_{cm})^2\) is replaced by \((r_{ix} - r_{cxm}) * (r_{iy} - r_{cmy})\) for the xy component, etc. The 6 components of the tensor are ordered xx, yy, zz, xy, xz, yz.

\( R_g \) for a particular molecule is only computed if one or more of its atoms are in the specified group. Normally all atoms in the molecule should be in the group, however this is not required. LAMMPS will warn you if this is not the case. Only atoms in the group contribute to the \( R_g \) calculation for the molecule.

The ordering of per-molecule quantities produced by this compute is consistent with the ordering produced by other compute commands that generate per-molecule datums. Conceptually, them molecule IDs will be in ascending order for any molecule with one or more of its atoms in the specified group.

IMPORTANT NOTE: The coordinates of an atom contribute to \( R_g \) in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.
Output info:

This compute calculates a global vector if the tensor keyword is not specified and a global array if it is. The length of the vector or number of rows in the array is the number of molecules. If the tensor keyword is specified, the global array has 6 columns. The vector or array can be accessed by any command that uses global values from a compute as input. See this section for an overview of LAMMPS output options.

All the vector or array values calculated by this compute are "intensive". The vector or array values will be in distance units.

Restrictions: none

Related commands: none

compute gyration

Default: none
**compute heat/flux command**

**Syntax:**

compute ID group-ID heat/flux ke-ID pe-ID stress-ID

- ID, group-ID are documented in `compute` command
- heat/flux = style name of this compute command
- ke-ID = ID of a compute that calculates per-atom kinetic energy
- pe-ID = ID of a compute that calculates per-atom potential energy
- stress-ID = ID of a compute that calculates per-atom stress

**Examples:**

compute myFlux all heat/flux myKE myPE myStress

**Description:**

Define a computation that calculates the heat flux vector based on contributions from atoms in the specified group. This can be used by itself to measure the heat flux into or out of a reservoir of atoms, or to calculate a thermal conductivity using the Green-Kubo formalism.

See the `fix thermal/conductivity` command for details on how to compute thermal conductivity in an alternate way, via the Muller-Plathe method. See the `fix heat` command for a way to control the heat added or subtracted to a group of atoms.

The compute takes three arguments which are IDs of other `computes`. One calculates per-atom kinetic energy (`ke-ID`), one calculates per-atom potential energy (`pe-ID`), and the third calculates per-atom stress (`stress-ID`). These should be defined for the same group used by `compute heat/flux`, though LAMMPS does not check for this.

The Green-Kubo formulas relate the ensemble average of the auto-correlation of the heat flux $J$ to the thermal conductivity $\kappa$:

\[
J = \frac{1}{V} \left[ \sum_i e_i v_i - \sum_i s_i v_i \right]
\]

\[
= \frac{1}{V} \left[ \sum_i e_i v_i + \sum_{i<j} (f_{ij} \cdot v_j) x_{ij} \right]
\]

\[
= \frac{1}{V} \left[ \sum_i e_i v_i + \frac{1}{2} \sum_{i<j} (f_{ij} \cdot (v_i + v_j)) x_{ij} \right]
\]
\[ \kappa = \frac{V}{k_B T^2} \int_0^\infty \langle J_x(0)J_x(t) \rangle \, dt = \frac{V}{3k_B T^2} \int_0^\infty \langle \mathbf{J}(0) \cdot \mathbf{J}(t) \rangle \, dt \]

Ei in the first term of the equation for \( J \) is the per-atom energy (potential and kinetic). This is calculated by the computes \( ke-ID \) and \( pe-ID \). Si in the second term of the equation for \( J \) is the per-atom stress tensor calculated by the compute \( stress-ID \). The tensor multiplies \( \mathbf{V} \) as a 3x3 matrix-vector multiply to yield a vector. Note that as discussed below, the \( 1/V \) scaling factor in the equation for \( J \) is NOT included in the calculation performed by this compute; you need to add it for a volume appropriate to the atoms included in the calculation.

IMPORTANT NOTE: The compute pe/atom and compute stress/atom commands have options for which terms to include in their calculation (pair, bond, etc). The heat flux calculation will thus include exactly the same terms. Normally you should use compute stress/atom virial so as not to include a kinetic energy term in the heat flux.

This compute calculates 6 quantities and stores them in a 6-component vector. The first 3 components are the \( x, y, z \) components of the full heat flux vector, i.e. \( (J_x, J_y, J_z) \). The next 3 components are the \( x, y, z \) components of just the convective portion of the flux, i.e. the first term in the equation for \( J \) above.

The heat flux can be output every so many timesteps (e.g. via the thermo_style custom command). Then as a post-processing operation, an autocorrelation can be performed, its integral estimated, and the Green-Kubo formula above evaluated.

The fix ave/correlate command can calculate the autocorrelation. The trap() function in the variable command can calculate the integral.

An example LAMMPS input script for solid Ar is appended below. The result should be: average conductivity \(~0.29\) in W/mK.

Output info:

This compute calculates a global vector of length 6 (total heat flux vector, followed by conductive heat flux vector), which can be accessed by indices 1-6. These values can be used by any command that uses global vector values from a compute as input. See this section for an overview of LAMMPS output options.

The vector values calculated by this compute are "extensive", meaning they scale with the number of atoms in the simulation. They can be divided by the appropriate volume to get a flux, which would then be an "intensive" value, meaning independent of the number of atoms in the simulation. Note that if the compute is "all", then the appropriate volume to divide by is the simulation box volume. However, if a sub-group is used, it should be the volume containing those atoms.

The vector values will be in energy*velocity units. Once divided by a volume the units will be that of flux, namely energy/area/time units

Restrictions: none

Related commands:

fix thermal/conductivity, fix ave/correlate, variable

Default: none
# Sample LAMMPS input script for thermal conductivity of solid Ar

units       real
variable    T equal 70
variable    V equal vol
variable    dt equal 4.0
variable    p equal 200   # correlation length
variable    s equal 10    # sample interval
variable    d equal $p*$s   # dump interval

# convert from LAMMPS real units to SI

variable    kB equal 1.3806504e-23    # [J/K] Boltzmann
variable    kCal2J equal 4186.0/6.02214e23
variable    A2m equal 1.0e-10
variable    fs2s equal 1.0e-15
variable    convert equal ${kCal2J}*${kB}/$V*$s*${dt}*

# setup problem

dimension    3
boundary     p p p
lattice      fcc 5.376 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       box block 0 4 0 4 0 4
create_box   1 box
create_atoms 1 box
mass         1 39.948
pair_style   lj/cut 13.0
pair_coeff   * * 0.2381 3.405

velocity     all create $T 102486 mom yes rot yes dist gaussian
fix          NVT all nvt temp $T $T 10 drag 0.2
run          8000

# thermal conductivity calculation, switch to NVE if desired

#unfix       NVT
#fix         NVE all nve

reset_timestep 0
compute      myKE all ke/atom
compute      myPE all pe/atom
compute      myStress all stress/atom virial
compute      flux all heat/flux myKE myPE myStress
variable    Jx equal c_flux[1]/vol
variable    Jy equal c_flux[2]/vol
variable    Jz equal c_flux[3]/vol
fix          JJ all ave/correlate $s $p $d &
variable    scale equal $(convert)/${kB}/$T/$V*$s*${dt}*

variable    k11 equal trap(f_JJ[3])*${scale}
variable    k22 equal trap(f_JJ[4])*${scale}
variable    k33 equal trap(f_JJ[5])*${scale}

thermo_style custom step temp v_Jx v_Jy v_Jz v_k11 v_k22 v_k33
run          100000
variable    k equal (v_k11+v_k22+v_k33)/3.0
variable    ndens equal count(all)/vol
print        "average conductivity: $k[W/mK] @ $T K, $\text{dens} /A^3"
compute improper/local command

Syntax:

compute ID group-ID improper/local input1 input2 ...

- ID, group-ID are documented in compute command
- improper/local = style name of this compute command
- zero or more keywords may be appended
- keyword = chi

chi = tabulate improper angles

Examples:

compute 1 all improper/local chi

Description:

Define a computation that calculates properties of individual improper interactions. The number of datums generated, aggregated across all processors, equals the number of impropers in the system.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their impropers. An improper will only be included if all 4 atoms in the improper are in the specified compute group.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, improper output from the compute property/local command can be combined with data from this command and output by the dump local command in a consistent way.

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of impropers. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The output for chi will be in degrees.

Restrictions: none

Related commands:

dump local, compute property/local

Default: none
**compute ke command**

**Syntax:**

```plaintext
compute ID group-ID ke
```

- ID, group-ID are documented in `compute` command
- `ke` = style name of this compute command

**Examples:**

```plaintext
compute 1 all ke
```

**Description:**

Define a computation that calculates the translational kinetic energy of a group of particles.

The kinetic energy of each particle is computed as \( \frac{1}{2} m v^2 \), where \( m \) and \( v \) are the mass and velocity of the particle.

There is a subtle difference between the quantity calculated by this compute and the kinetic energy calculated by the `ke` or `etotal` keyword used in thermodynamic output, as specified by the `thermo_style` command. For this compute, kinetic energy is "translational" kinetic energy, calculated by the simple formula above. For thermodynamic output, the `ke` keyword infers kinetic energy from the temperature of the system with \( \frac{1}{2} k_B T \) of energy for each degree of freedom. For the default temperature computation via the `compute temp` command, these are the same. But different computes that calculate temperature can subtract out different non-thermal components of velocity and/or include different degrees of freedom (translational, rotational, etc).

**Output info:**

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See Section howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

**Restrictions:** none

**Related commands:**

- `compute erotate/sphere`

**Default:** none
compute ke/atom command

Syntax:

compute ID group-ID ke/atom

- ID, group-ID are documented in compute command
- ke/atom = style name of this compute command

Examples:

compute 1 all ke/atom

Description:

Define a computation that calculates the per-atom translational kinetic energy for each atom in a group. The kinetic energy is simply 1/2 m v^2, where m is the mass and v is the velocity of each atom. The value of the kinetic energy will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions: none

Related commands:

dump custom

Default: none
compute ke/atom/eff command

Syntax:

compute ID group-ID ke/atom/eff

- ID, group-ID are documented in compute command
- ke/atom/eff = style name of this compute command

Examples:

compute 1 all ke/atom/eff

Description:

Define a computation that calculates the per-atom translational (nuclei and electrons) and radial kinetic energy (electron only) in a group. The particles are assumed to be nuclei and electrons modeled with the electronic force field.

The kinetic energy for each nucleus is computed as 1/2 m v^2, where m corresponds to the corresponding nuclear mass, and the kinetic energy for each electron is computed as 1/2 (me v^2 + 3/4 me s^2), where me and v correspond to the mass and translational velocity of each electron, and s to its radial velocity, respectively.

There is a subtle difference between the quantity calculated by this compute and the kinetic energy calculated by the \textit{ke} or \textit{etotal} keyword used in thermodynamic output, as specified by the \texttt{thermo\_style} command. For this compute, kinetic energy is "translational" plus electronic "radial" kinetic energy, calculated by the simple formula above. For thermodynamic output, the \textit{ke} keyword infers kinetic energy from the temperature of the system with 1/2 Kb T of energy for each (nuclear-only) degree of freedom in eFF.

\textbf{IMPORTANT NOTE:} The temperature in eFF should be monitored via the compute temp/eff command, which can be printed with thermodynamic output by using the \texttt{thermo\_modify} command, as shown in the following example:

```
compute         effTemp all temp/eff
thermo_style    custom step etotal pe ke temp press
thermo_modify   temp effTemp
```

The value of the kinetic energy will be 0.0 for atoms (nuclei or electrons) not in the specified compute group.

Output info:

This compute calculates a scalar quantity for each atom, which can be accessed by any command that uses per-atom computes as input. See \texttt{Section\_howto 15} for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions:

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the \texttt{Making LAMMPS} section for more info.
Related commands:

dump custom

Default: none
compute ke/eff command

Syntax:

compute ID group-ID ke/eff

• ID, group-ID are documented in compute command
• ke/eff = style name of this compute command

Examples:

compute 1 all ke/eff

Description:

Define a computation that calculates the kinetic energy of motion of a group of eFF particles (nuclei and electrons), as modeled with the electronic force field.

The kinetic energy for each nucleus is computed as 1/2 m v^2 and the kinetic energy for each electron is computed as 1/2(me v^2 + 3/4 me s^2), where m corresponds to the nuclear mass, me to the electron mass, v to the translational velocity of each particle, and s to the radial velocity of the electron, respectively.

There is a subtle difference between the quantity calculated by this compute and the kinetic energy calculated by the ke or etotal keyword used in thermodynamic output, as specified by the thermo_style command. For this compute, kinetic energy is "translational" and "radial" (only for electrons) kinetic energy, calculated by the simple formula above. For thermodynamic output, the ke keyword infers kinetic energy from the temperature of the system with 1/2 Kb T of energy for each degree of freedom. For the eFF temperature computation via the compute temp/eff command, these are the same. But different computes that calculate temperature can subtract out different non-thermal components of velocity and/or include other degrees of freedom.

IMPORTANT NOTE: The temperature in eFF models should be monitored via the compute temp/eff command, which can be printed with thermodynamic output by using the thermo_modify command, as shown in the following example:

compute         effTemp all temp/eff
thermo_style    custom step etotal pe ke temp press
thermo_modify   temp effTemp

See compute temp/eff.

Output info:

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions:

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.
Related commands: none

Default: none
compute meso_e/atom command

Syntax:
compute ID group-ID meso_e/atom

• ID, group-ID are documented in compute command
• meso_e/atom = style name of this compute command

Examples:
compute 1 all meso_e/atom

Description:
Define a computation that calculates the per-atom internal energy for each atom in a group.

The internal energy is the energy associated with the internal degrees of freedom of a mesoscopic particles, e.g. a Smooth-Particle Hydrodynamics particle.

See this PDF guide to using SPH in LAMMPS.

The value of the internal energy will be 0.0 for atoms not in the specified compute group.

Output info:
This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions:
This compute is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:
dump custom

Default: none
compute meso_rho/atom command

Syntax:
compute ID group-ID meso_rho/atom

- ID, group-ID are documented in compute command
- meso_rho/atom = style name of this compute command

Examples:
compute 1 all meso_rho/atom

Description:
Define a computation that calculates the per-atom mesoscopic density for each atom in a group.

The mesoscopic density is the mass density of a mesoscopic particle, calculated by kernel function interpolation using "pair style sph/rhosum".

See this PDF guide to using SPH in LAMMPS.

The value of the mesoscopic density will be 0.0 for atoms not in the specified compute group.

Output info:
This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in mass/volume units.

Restrictions:
This compute is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:
dump custom

Default: none
compute meso_t/atom command

Syntax:

compute ID group-ID meso_t/atom

- ID, group-ID are documented in compute command
- meso_t/atom = style name of this compute command

Examples:

compute 1 all meso_t/atom

Description:

Define a computation that calculates the per-atom internal temperature for each atom in a group.

The internal temperature is the ratio of internal energy over the heat capacity associated with the internal degrees of freedom of a mesoscopic particles, e.g. a Smooth-Particle Hydrodynamics particle.

\[ T_{\text{int}} = \frac{E_{\text{int}}}{C_{\text{V, int}}} \]

See this PDF guide to using SPH in LAMMPS.

The value of the internal energy will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in temperature units.

Restrictions:

This compute is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

dump custom

Default: none
compute_modify command

Syntax:

```
compute_modify compute-ID keyword value ...
```

- compute-ID = ID of the compute to modify
- one or more keyword/value pairs may be listed
- keyword = extra or dynamic

extra value = N
  N = # of extra degrees of freedom to subtract
dynamic value = yes or no
  yes/no = do or do not recompute the number of atoms contributing to the temperature
thermo value = yes or no
  yes/no = do or do not add contributions from fixes to the potential energy

Examples:

```
compute_modify myTemp extra 0
compute_modify newtemp dynamic yes extra 600
```

Description:

Modify one or more parameters of a previously defined compute. Not all compute styles support all parameters.

The extra keyword refers to how many degrees-of-freedom are subtracted (typically from 3N) as a normalizing factor in a temperature computation. Only computes that compute a temperature use this option. The default is 2 or 3 for 2d or 3d systems which is a correction factor for an ensemble of velocities with zero total linear momentum. You can use a negative number for the extra parameter if you need to add degrees-of-freedom. See the compute temp/asphere command for an example.

The dynamic keyword determines whether the number of atoms N in the compute group is re-computed each time a temperature is computed. Only compute styles that compute a temperature use this option. By default, N is assumed to be constant. If you are adding atoms to the system (see the fix pour or fix deposit commands) or expect atoms to be lost (e.g. due to evaporation), then this option can be used to insure the temperature is correctly normalized.

The thermo keyword determines whether the potential energy contribution calculated by some fixes is added to the potential energy calculated by the compute. Currently, only the compute of style pe uses this option. See the doc pages for individual fixes for details.

Restrictions: none

Related commands:

compute

Default:

The option defaults are extra = 2 or 3 for 2d or 3d systems and dynamic = no. Thermo is yes if the compute of style pe was defined with no extra keywords; otherwise it is no.
compute msd command

Syntax:

compute ID group-ID msd keyword values ...

- ID, group-ID are documented in compute command
- msd = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = com

  com value = yes or no

Examples:

compute 1 all msd
compute 1 upper msd com yes

Description:

Define a computation that calculates the mean-squared displacement (MSD) of the group of atoms, including all effects due to atoms passing thru periodic boundaries.

A vector of four quantities is calculated by this compute. The first 3 elements of the vector are the squared dx,dy,dz displacements, summed and averaged over atoms in the group. The 4th component is the total squared displacement, i.e. (dx*dx + dy*dy + dz*dz), summed and averaged over atoms in the group.

The slope of the mean-squared displacement (MSD) versus time is proportional to the diffusion coefficient of the diffusing atoms.

The displacement of an atom is from its original position at the time the compute command was issued. To store the original coordinates, the compute creates its own fix of style "store/state", as if this command had been issued:

fix compute-ID_store_state group-ID store/state xu yu zu

See the fix store/state command for details. Note that the ID of the new fix is the compute-ID + underscore + "store_state", and the group for the new fix is the same as the compute group.

If the com option is set to yes then the effect of any drift in the center-of-mass of the group of atoms is subtracted out before the displacement of each atom is calculated. The com option is also passed to the created fix store/state.

IMPORTANT NOTE: Fix store/state stores the initial coordinates in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

IMPORTANT NOTE: If an atom is part of a rigid body (see the fix rigid command), it's periodic image flags are altered, and its contribution to the MSD may not reflect its true contribution. See the fix rigid command for details. Thus, to compute the MSD of rigid bodies as they cross periodic boundaries, you will need to post-process a dump file containing coordinates of the atoms in the bodies.
IMPORTANT NOTE: If you want the quantities calculated by this compute to be continuous when running from a restart file, then you should use the same ID for this compute, as in the original run. This is so that the created fix will also have the same ID, and thus be initialized correctly with atom coordinates from the restart file.

Output info:

This compute calculates a global vector of length 4, which can be accessed by indices 1-4 by any command that uses global vector values from a compute as input. See this section for an overview of LAMMPS output options.

The vector values are "intensive". The vector values will be in distance^2 units.

Restrictions: none

Related commands:

compute displace_atom, fix store/state, compute msd/molecule

Default:

The option default is com = no.
compute msd/molecule command

Syntax:

compute ID group-ID msd/molecule

- ID, group-ID are documented in compute command
- msd/molecule = style name of this compute command

Examples:

compute 1 all msd/molecule

Description:

Define a computation that calculates the mean-squared displacement (MSD) of individual molecules. The calculation includes all effects due to atoms passing thru periodic boundaries.

Four quantities are calculated by this compute for each molecule. The first 3 quantities are the squared dx,dy,dz displacements of the center-of-mass. The 4th component is the total squared displacement, i.e. \((dx*dx + dy*dy + dz*dz)\) of the center-of-mass.

The slope of the mean-squared displacement (MSD) versus time is proportional to the diffusion coefficient of the diffusing molecules.

The displacement of the center-of-mass of the molecule is from its original center-of-mass position at the time the compute command was issued.

The MSD for a particular molecule is only computed if one or more of its atoms are in the specified group. Normally all atoms in the molecule should be in the group, however this is not required. LAMMPS will warn you if this is not the case. Only atoms in the group contribute to the center-of-mass calculation for the molecule, which is used to calculate its initial and current position.

The ordering of per-molecule quantities produced by this compute is consistent with the ordering produced by other compute commands that generate per-molecule datums. Conceptually, these molecule IDs will be in ascending order for any molecule with one or more of its atoms in the specified group.

IMPORTANT NOTE: The initial coordinates of each molecule are stored in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

IMPORTANT NOTE: If an atom is part of a rigid body (see the fix rigid command), its periodic image flags are altered, and its contribution to the MSD may not reflect its true contribution. See the fix rigid command for details. Thus, to compute the MSD of rigid bodies as they cross periodic boundaries, you will need to post-process a dump file containing coordinates of the atoms in the bodies.

IMPORTANT NOTE: Unlike the compute msd command, this compute does not store the initial center-of-mass coordinates of its molecules in a restart file. Thus you cannot continue the MSD per molecule calculation of this
compute when running from a restart file.

Output info:

This compute calculates a global array where the number of rows = Nmolecules and the number of columns = 4 for dx,dy,dz and the total displacement. These values can be accessed by any command that uses global array values from a compute as input. See this section for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in distance^2 units.

Restrictions: none

Related commands:

compute msd

Default: none
**compute pair command**

**Syntax:**

```
compute ID group-ID pair pstyle evalue
```

- **ID, group-ID** are documented in `compute` command
- **pair** = style name of this compute command
- **pstyle** = style name of a pair style that calculates additional values
- **evalue** = `epair` or `evdwl` or `ecoul` or blank (optional setting)

**Examples:**

```
compute 1 all pair gauss
compute 1 all pair lj/cut/coul/cut ecoul
compute 1 all pair reax
```

**Description:**

Define a computation that extracts additional values calculated by a pair style, sums them across processors, and makes them accessible for output or further processing by other commands. The group specified for this command is ignored.

The specified `pstyle` must be a pair style used in your simulation either by itself or as a sub-style in a `pair_style hybrid` or `hybrid/overlay` command.

The `evalue` setting is optional; it may be left off the command. All pair styles tally a potential energy `epair` which may be broken into two parts: `evdwl` and `ecoul` such that `epair = evdwl + ecoul`. If the pair style calculates Coulombic interactions, their energy will be tallied in `ecoul`. Everything else (whether it is a Lennard-Jones style van der Waals interaction or not) is tallied in `evdwl`. If `evalue` is specified as `epair` or left out, then `epair` is stored as a global scalar by this compute. This is useful when using `pair_style hybrid` if you want to know the portion of the total energy contributed by one sub-style. If `evalue` is specified as `evdwl` or `ecoul`, then just that portion of the energy is stored as a global scalar.

Some pair styles tally additional quantities, e.g. a breakdown of potential energy into a dozen or so components is tallied by the `pair_style reax` command. These values (1 or more) are stored as a global vector by this compute. See the doc page for individual `pair styles` for info on these values.

**Output info:**

This compute calculates a global scalar which is `epair` or `evdwl` or `ecoul`. If the pair style supports it, it also calculates a global vector of length >= 1, as determined by the pair style. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar and vector values calculated by this compute are "extensive".

The scalar value will be in energy units. The vector values will typically also be in energy units, but see the doc page for the pair style for details.

**Restrictions:** none
Related commands:

compute pe

Default:

The default for evaluate is epair.
compute pair/local command

Syntax:

compute ID group-ID pair/local input1 input2 ...

- ID, group-ID are documented in compute command
- pair/local = style name of this compute command
- zero or more keywords may be appended
- keyword = dist or eng or force or fx or fy or fz or pN

\[\text{dist} = \text{pairwise distance} \]
\[\text{eng} = \text{pairwise energy} \]
\[\text{force} = \text{pairwise force} \]
\[\text{fx, fy, fz} = \text{components of pairwise force} \]
\[\text{pN} = \text{pair style specific quantities for allowed N values} \]

Examples:

compute 1 all pair/local eng
compute 1 all pair/local dist eng force
compute 1 all pair/local dist eng fx fy fz
compute 1 all pair/local dist fx fy fz p1 p2 p3

Description:

Define a computation that calculates properties of individual pairwise interactions. The number of datums generated, aggregated across all processors, equals the number of pairwise interactions in the system.

The local data stored by this command is generated by looping over the pairwise neighbor list. Info about an individual pairwise interaction will only be included if both atoms in the pair are in the specified compute group, and if the current pairwise distance is less than the force cutoff distance for that interaction, as defined by the pair_style and pair_coeff commands.

The output dist is the distance between the pair of atoms.

The output eng is the interaction energy for the pair of atoms.

The output force is the force acting between the pair of atoms, which is positive for a repulsive force and negative for an attractive force. The outputs fx, fy, and fz are the xyz components of force on atom I.

A pair style may define additional pairwise quantities which can be accessed as p1 to pN, where N is defined by the pair style. Most pair styles do not define any additional quantities, so N = 0. An example of ones that do are the granular pair styles which calculate the tangential force between two particles and return its components and magnitude acting on atom I for N = 1,2,3,4. See individual pair styles for details.

The output dist will be in distance units. The output eng will be in energy units. The outputs force, fx, fy, and fz will be in force units. The output pN will be in whatever units the pair style defines.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For
example, pair output from the `compute property/local` command can be combined with data from this command and output by the `dump local` command in a consistent way.

IMPORTANT NOTE: For pairs, if two atoms I,J are involved in 1-2, 1-3, 1-4 interactions within the molecular topology, their pairwise interaction may be turned off, and thus they may not appear in the neighbor list, and will not be part of the local data created by this command. More specifically, this may be true of I,J pairs with a weighting factor of 0.0; pairs with a non-zero weighting factor are included. The weighting factors for 1-2, 1-3, and 1-4 pairwise interactions are set by the `special_bonds` command.

**Output info:**

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of pairs. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See [this section](#) for an overview of LAMMPS output options.

The output for `dist` will be in distance [units](#). The output for `eng` will be in energy [units](#). The output for `force` will be in force [units](#).

**Restrictions:** none

**Related commands:**

dump local, compute property/local

**Default:** none
compute pe command

compute pe/cuda command

Syntax:

compute ID group-ID pe keyword ...

- ID, group-ID are documented in compute command
- pe = style name of this compute command
- zero or more keywords may be appended
- keyword = pair or bond or angle or dihedral or improper or kspace

Examples:

compute 1 all pe
compute molPE all pe bond angle dihedral improper

Description:

Define a computation that calculates the potential energy of the entire system of atoms. The specified group must be "all". See the compute pe/atom command if you want per-atom energies. These per-atom values could be summed for a group of atoms via the compute reduce command.

The energy is calculated by the various pair, bond, etc potentials defined for the simulation. If no extra keywords are listed, then the potential energy is the sum of pair, bond, angle, dihedral, improper, and kspace (long-range) energy. If any extra keywords are listed, then only those components are summed to compute the potential energy.

The Kspace contribution requires 1 extra FFT each timestep the energy is calculated, if using the PPPM solver via the kspace_style pppm command. Thus it can increase the cost of the PPPM calculation if it is needed on a large fraction of the simulation timesteps.

Various fixes can contribute to the total potential energy of the system. See the doc pages for individual fixes for details. The thermo option of the compute_modify command determines whether these contributions are added into the computed potential energy. If no keywords are specified the default is yes. If any keywords are specified, the default is no.

A compute of this style with the ID of "thermo_pe" is created when LAMMPS starts up, as if this command were in the input script:

compute thermo_pe all pe

See the "thermo_style" command for more details.

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.
These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Output info:**

This compute calculates a global scalar (the potential energy). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

**Restrictions:** none

**Related commands:**

compute pe/atom

**Default:** none
compute pe/atom command

Syntax:

compute ID group-ID pe/atom keyword ... 

- ID, group-ID are documented in compute command
- pe/atom = style name of this compute command
- zero or more keywords may be appended
- keyword = pair or bond or angle or dihedral or improper or kspace

Examples:

compute 1 all pe/atom
compute 1 all pe/atom pair
compute 1 all pe/atom pair bond

Description:

Define a computation that computes the per-atom potential energy for each atom in a group. See the compute pe command if you want the potential energy of the entire system.

The per-atom energy is calculated by the various pair, bond, etc potentials defined for the simulation. If no extra keywords are listed, then the potential energy is the sum of pair, bond, angle, dihedral,improper, and kspace energy. If any extra keywords are listed, then only those components are summed to compute the potential energy.

Note that the energy of each atom is due to its interaction with all other atoms in the simulation, not just with other atoms in the group.

For an energy contribution produced by a small set of atoms (e.g. 4 atoms in a dihedral or 3 atoms in a Tersoff 3-body interaction), that energy is assigned in equal portions to each atom in the set. E.g. 1/4 of the dihedral energy to each of the 4 atoms.

The dihedral_style charmm style calculates pairwise interactions between 1-4 atoms. The energy contribution of these terms is included in the pair energy, not the dihedral energy.

The KSpace contribution is calculated using the method in (Heyes) for the Ewald method and a related method for PPPM, as specified by the kspace_style ppm command. For PPPM, the calculation requires 1 extra FFT each timestep that per-atom energy is calculated. This document describes how the long-range per-atom energy calculation is performed.

As an example of per-atom potential energy compared to total potential energy, these lines in an input script should yield the same result in the last 2 columns of thermo output:

compute peratom all pe/atom
compute pe all reduce sum c_peratom
thermo_style custom step temp etotal press pe c_pe

IMPORTANT NOTE: The per-atom energy does not any Lennard-Jones tail corrections invoked by the pair_modify tail yes command, since those are global contributions to the system energy.
Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions:

Related commands:

compute pe, compute stress/atom

Default: none

(Heyes) Heyes, Phys Rev B 49, 755 (1994),
compute pressure command

compute pressure/cuda command

Syntax:

compute ID group-ID pressure temp-ID keyword ...

- ID, group-ID are documented in compute command
- pressure = style name of this compute command
- temp-ID = ID of compute that calculates temperature
- zero or more keywords may be appended
- keyword = ke or pair or bond or angle or dihedral or improper or kspace or fix or virial

Examples:

compute 1 all pressure myTemp
compute 1 all pressure thermo_temp pair bond

Description:

Define a computation that calculates the pressure of the entire system of atoms. The specified group must be "all". See the compute stress/atom command if you want per-atom pressure (stress). These per-atom values could be summed for a group of atoms via the compute reduce command.

The pressure is computed by the formula

\[ P = \frac{N k_B T}{V} + \sum_i \frac{r_i \cdot f_i}{dV} \]

where N is the number of atoms in the system (see discussion of DOF below), Kb is the Boltzmann constant, T is the temperature, d is the dimensionality of the system (2 or 3 for 2d/3d), V is the system volume (or area in 2d), and the second term is the virial, computed within LAMMPS for all pairwise as well as 2-body, 3-body, and 4-body, and long-range interactions. Fixes that impose constraints (e.g. the fix shake command) also contribute to the virial term.

A symmetric pressure tensor, stored as a 6-element vector, is also calculated by this compute. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz. The equation for the I,J components (where I and J = x,y,z) is similar to the above formula, except that the first term uses components of the kinetic energy tensor and the second term uses components of the virial tensor:

\[ P_{IJ} = \frac{\sum_k m_k v_{kI} v_{kJ}}{V} + \frac{\sum_k r_{kI} f_{kJ}}{V} \]
If no extra keywords are listed, the entire equations above are calculated which include a kinetic energy (temperature) term and the virial as the sum of pair, bond, angle, dihedral, improper, kspace (long-range), and fix contributions to the force on each atom. If any extra keywords are listed, then only those components are summed to compute temperature or ke and/or the virial. The virial keyword means include all terms except the kinetic energy \( ke \).

The temperature and kinetic energy tensor is not calculated by this compute, but rather by the temperature compute specified with the command. Normally this compute should calculate the temperature of all atoms for consistency with the virial term, but any compute style that calculates temperature can be used, e.g. one that excludes frozen atoms or other degrees of freedom.

Note that the \( N \) in the first formula above is really degrees-of-freedom divided by \( d = \) dimensionality, where the DOF value is calculated by the temperature compute. See the various compute temperature styles for details.

A compute of this style with the ID of "thermo_press" is created when LAMMPS starts up, as if this command were in the input script:

```
compute thermo_press all pressure thermo_temp
```

where "thermo_temp" is the ID of a similarly defined compute of style "temp". See the "thermo_style" command for more details.

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Output info:**

This compute calculates a global scalar (the pressure) and a global vector of length 6 (pressure tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar and vector values calculated by this compute are "intensive". The scalar and vector values will be in pressure units.

**Restrictions:** none

**Related commands:**

compute temp, compute stress/atom, thermo_style,

**Default:** none
compute property/atom command

Syntax:

compute ID group-ID property/atom input1 input2 ...

- ID, group-ID are documented in compute command
- property/atom = style name of this compute command
- input = one or more atom attributes

possible attributes = id, mol, type, mass, x, y, z, xs, ys, zs, xu, yu, zu, ix, iy, iz, vx, vy, vz, fx, fy, fz, q, mux, muy, muz, mu, radius, diameter, omegax, omegay, omegaz, angmomx, anngomy, angmomz, shapex, shapey, shapez, quatw, quati, quatj, quatk, tqx, tqty, tqz, spin, eradius, ervel, erforce, end1x, endly, end1z, end2x, end2y, end2z, corner1x, cornerly, corner1z, corner2x, corner2y, corner2z, corner3x, corner3y, corner3z

id = atom ID
mol = molecule ID
type = atom type
mass = atom mass
x, y, z = unscaled atom coordinates
xs, ys, zs = scaled atom coordinates
xu, yu, zu = unwrapped atom coordinates
ix, iy, iz = box image that the atom is in
vx, vy, vz = atom velocities
fx, fy, fz = forces on atoms
q = atom charge
mux, muy, muz = orientation of dipole moment of atom
mu = magnitude of dipole moment of atom
radius, diameter = radius, diameter of spherical particle
omegax, omegay, omegaz = angular velocity of extended particle
angmomx, angmom, angmomz = angular momentum of extended particle
shapex, shapey, shapez = 3 diameters of aspherical particle
quatw, quati, quatj, quatk = quaternion components for aspherical particles
tqx, tqty, tqz = torque on extended particles
spin = electron spin
eradius = electron radius
ervel = electron radial velocity
erforce = electron radial force
end12x, end12y, end12z = end points of line segment
corner123x, corner123y, corner123z = corner points of triangle

Examples:

compute 1 all property/atom xs vx fx mux
compute 2 all property/atom type
compute 1 all property/atom ix iy iz

Description:
Define a computation that simply stores atom attributes for each atom in the group. This is useful so that the values can be used by other output commands that take computes as inputs. See for example, the compute reduce, fix ave/atom, fix ave/histo, fix ave/spatial, and atom-style variable commands.

The list of possible attributes is the same as that used by the dump custom command, which describes their meaning, with some additional quantities that are only defined for certain atom styles. Basically, this list gives your input script access to any per-atom quantity stored by LAMMPS.

The values are stored in a per-atom vector or array as discussed below. Zeroes are stored for atoms not in the specified group or for quantities that are not defined for a particular particle in the group (e.g. shapex if the particle is not an ellipsoid).

The additional quantities only accessible via this command, and not directly via the dump custom command, are as follows.

Shapex, shapey, and shapez are defined for ellipsoidal particles and define the 3d shape of each particle. Quatw, quati, quatj, and quatk are also defined for ellipsoidal particles and store the 4-vector quaternion representing the orientation of each particle. See the set command for an explanation of the quaternion vector.

End1x, end1y, end1z, end2x, end2y, end2z, are defined for line segment particles and define the end points of each line segment.

Corner1x, corner1y, corner1z, corner2x, corner2y, corner2z, corner3x, corner3y, corner3z, are defined for triangular particles and define the corner points of each triangle.

Output info:

This compute calculates a per-atom vector or per-atom array depending on the number of input values. If a single input is specified, a per-atom vector is produced. If two or more inputs are specified, a per-atom array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses per-atom values from a compute as input. See this section for an overview of LAMMPS output options.

The vector or array values will be in whatever units the corresponding attribute is in, e.g. velocity units for vx, charge units for q, etc.

Restrictions: none

Related commands:
dump custom, compute reduce, fix ave/atom, fix ave/spatial

Default: none
compute property/local command

Syntax:

compute ID group-ID property/local input1 input2 ...

• ID, group-ID are documented in compute command
• property/local = style name of this compute command
• input = one or more attributes

possible attributes = natom1 natom2 ntype1 ntype2
patom1 patom2 ptype1 ptype2
batom1 batom2 btype
aatom1 aatom2 aatom3 atype
datom1 datom2 datom3 dtype
iatom1 iatom2 iatom3 itype

natom1, natom2 = IDs of 2 atoms in each pair (within neighbor cutoff)
ntype1, ntype2 = type of 2 atoms in each pair (within neighbor cutoff)
patom1, patom2 = IDs of 2 atoms in each pair (within force cutoff)
ptype1, ptype2 = type of 2 atoms in each pair (within force cutoff)
batom1, batom2 = IDs of 2 atoms in each bond
btype = bond type of each bond
aatom1, aatom2, aatom3 = IDs of 3 atoms in each angle
atype = angle type of each angle
datom1, datom2, datom3, datom4 = IDs of 4 atoms in each dihedral
dtype = dihedral type of each dihedral
iatom1, iatom2, iatom3, iatom4 = IDs of 4 atoms in each improper
itype = improper type of each improper

Examples:

compute 1 all property/local btype batom1 batom2
compute 1 all property/local atype aatom2

Description:

Define a computation that stores the specified attributes as local data so it can be accessed by other output commands. If the input attributes refer to bond information, then the number of datums generated, aggregated across all processors, equals the number of bonds in the system. Ditto for pairs, angles, etc.

If multiple input attributes are specified then they must all generate the same amount of information, so that the resulting local array has the same number of rows for each column. This means that only bond attributes can be specified together, or angle attributes, etc. Bond and angle attributes cannot be mixed in the same compute property/local command.

If the inputs are pair attributes, the local data is generated by looping over the pairwise neighbor list. Info about an individual pairwise interaction will only be included if both atoms in the pair are in the specified compute group. For natom1 and natom2, all atom pairs in the neighbor list are considered (out to the neighbor cutoff = force cutoff + neighbor skin). For patom1 and patom2, the distance between the atoms must be less than the force cutoff distance for that pair to be included, as defined by the pair_style and pair_coeff commands.

If the inputs are bond, angle, etc attributes, the local data is generated by looping over all the atoms owned on a processor and extracting bond, angle, etc info. For bonds, info about an individual bond will only be included if
both atoms in the bond are in the specified compute group. Likewise for angles, dihedrals, etc.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, output from the `compute bond/local` command can be combined with bond atom indices from this command and output by the `dump local` command in a consistent way.

The `natom1` and `natom2`, or `patom1` and `patom2` attributes refer to the atom IDs of the 2 atoms in each pairwise interaction computed by the `pair_style` command. The `ntype1` and `ntype2`, or `ptype1` and `ptype2` attributes refer to the atom types of the 2 atoms in each pairwise interaction.

**IMPORTANT NOTE:** For pairs, if two atoms I,J are involved in 1-2, 1-3, 1-4 interactions within the molecular topology, their pairwise interaction may be turned off, and thus they may not appear in the neighbor list, and will not be part of the local data created by this command. More specifically, this may be true of I,J pairs with a weighting factor of 0.0; pairs with a non-zero weighting factor are included. The weighting factors for 1-2, 1-3, and 1-4 pairwise interactions are set by the `special_bonds` command.

The `batom1` and `batom2` attributes refer to the atom IDs of the 2 atoms in each bond. The `btype` attribute refers to the type of the bond, from 1 to Nbtypes = # of bond types. The number of bond types is defined in the data file read by the `read_data` command.

The attributes that start with "a", "d", "i", refer to similar values for angles, dihedrals, and impropers.

**Output info:**

This compute calculates a local vector or local array depending on the number of input values. The length of the vector or number of rows in the array is the number of bonds, angles, etc. If a single input is specified, a local vector is produced. If two or more inputs are specified, a local array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The vector or array values will be integers that correspond to the specified attribute.

**Restrictions:** none

**Related commands:**

`dump local`, `compute reduce`

**Default:** none
compute property/molecule command

Syntax:

compute ID group-ID property/molecule input1 input2 ...

- ID, group-ID are documented in compute command
- property/molecule = style name of this compute command
- input = one or more attributes

possible attributes = mol cout
  mol = molecule ID
  count = # of atoms in molecule

Examples:

compute 1 all property/molecule mol

Description:

Define a computation that stores the specified attributes as global data so it can be accessed by other output commands and used in conjunction with other commands that generate per-molecule data, such as compute com/molecule and compute msd/molecule.

The ordering of per-molecule quantities produced by this compute is consistent with the ordering produced by other compute commands that generate per-molecule datums. Conceptually, them molecule IDs will be in ascending order for any molecule with one or more of its atoms in the specified group.

The mol attribute is the molecule ID. This attribute can be used to produce molecule IDs as labels for per-molecule datums generated by other computes or fixes when they are output to a file, e.g. by the fix ave/time command.

The count attribute is the number of atoms in the molecule.

Output info:

This compute calculates a global vector or global array depending on the number of input values. The length of the vector or number of rows in the array is the number of molecules. If a single input is specified, a global vector is produced. If two or more inputs are specified, a global array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses global values from a compute as input. See this section for an overview of LAMMPS output options.

The vector or array values will be integers that correspond to the specified attribute.

Restrictions: none

Related commands: none

Default: none
**compute rdf command**

**Syntax:**

```
compute ID group-ID rdf Nbin itype1 jtype1 itype2 jtype2 ...
```

- ID, group-ID are documented in `compute` command
- `rdf` = style name of this compute command
- `Nbin` = number of RDF bins
- `itypeN` = central atom type for Nth RDF histogram (see asterisk form below)
- `jtypeN` = distribution atom type for Nth RDF histogram (see asterisk form below)

**Examples:**

```
compute 1 all rdf 100
compute 1 all rdf 100 1 1
compute 1 all rdf 100 * 3
compute 1 fluid rdf 500 1 1 1 2 1 2 2
compute 1 fluid rdf 500 1*3 2 5 *10
```

**Description:**

Define a computation that calculates the radial distribution function (RDF), also called g(r), and the coordination number for a group of particles. Both are calculated in histogram form by binning pairwise distances into `Nbin` bins from 0.0 to the maximum force cutoff defined by the `pair_style` command. The bins are of uniform size in radial distance. Thus a single bin encompasses a thin shell of distances in 3d and a thin ring of distances in 2d.

The `itypeN` and `jtypeN` arguments are optional. These arguments must come in pairs. If no pairs are listed, then a single histogram is computed for g(r) between all atom types. If one or more pairs are listed, then a separate histogram is generated for each `itype,jtype` pair.

The `itypeN` and `jtypeN` settings can be specified in one of two ways. An explicit numeric value can be used, as in the 4th example above. Or a wild-card asterisk can be used to specify a range of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from n to n (inclusive).

If both `itypeN` and `jtypeN` are single values, as in the 4th example above, this means that a g(r) is computed where atoms of type `itypeN` are the central atom, and atoms of type `jtypeN` are the distribution atom. If either `itypeN` and `jtypeN` represent a range of values via the wild-card asterisk, as in the 5th example above, this means that a g(r) is computed where atoms of any of the range of types represented by `itypeN` are the central atom, and atoms of any of the range of types represented by `jtypeN` are the distribution atom.

Pairwise distances are generated by looping over a pairwise neighbor list, just as they would be in a `pair_style` computation. The distance between two atoms I and J is included in a specific histogram if the following criteria are met:

- atoms I,J are both in the specified compute group
- the distance between atoms I,J is less than the maximum force cutoff
- the type of the I atom matches `itypeN` (one or a range of types)
- the type of the J atom matches `jtypeN` (one or a range of types)
It is OK if a particular pairwise distance is included in more than one individual histogram, due to the way the `itypeN` and `jtypeN` arguments are specified.

The g(r) value for a bin is calculated from the histogram count by scaling it by the idealized number of how many counts there would be if atoms of type `jtypeN` were uniformly distributed. Thus it involves the count of `itypeN` atoms, the count of `jtypeN` atoms, the volume of the entire simulation box, and the volume of the bin's thin shell in 3d (or the area of the bin's thin ring in 2d).

A coordination number `coord(r)` is also calculated, which is the sum of g(r) values for all bins up to and including the current bin.

The simplest way to output the results of the compute rdf calculation to a file is to use the `fix ave/time` command, for example:

```
compute myRDF all rdf 50
fix 1 all ave/time 100 1 100 c_myRDF file tmp.rdf mode vector
```

**Output info:**

This compute calculates a global array with the number of rows = Nbins, and the number of columns = 1 + 2*Npairs, where Npairs is the number of I,J pairings specified. The first column has the bin coordinate (center of the bin). Each successive set of 2 columns has the g(r) and coord(r) values for a specific set of `itypeN` versus `jtypeN` interactions, as described above. These values can be used by any command that uses a global values from a compute as input. See Section _howto 15_ for an overview of LAMMPS output options.

The array values calculated by this compute are all "intensive".

The first column of array values will be in distance units. The g(r) columns of array values are normalized numbers >= 0.0. The coordination number columns of array values are also numbers >= 0.0.

**Restrictions:**

The RDF is not computed for distances longer than the force cutoff, since processors (in parallel) don't know about atom coordinates for atoms further away than that distance. If you want an RDF for larger distances, you can use the `rerun` command to post-process a dump file.

**Related commands:**

fix ave/time

**Default:** none
compute reduce command

compute reduce/region command

Syntax:

compute ID group-ID style arg mode input1 input2 ... keyword args ...  

- ID, group-ID are documented in compute command
- style = reduce or reduce/region

reduce arg = none
reduce/region arg = region-ID
region-ID = ID of region to use for choosing atoms
- mode = sum or min or max or ave
- one or more inputs can be listed
- input = x, y, z, vx, vy, vz, fx, fy, fz, c_ID, c_ID[N], f_ID, f_ID[N], v_name
  
x, y, z, vx, vy, vz, fx, fy, fz = atom attribute (position, velocity, force component)
c_ID = per-atom or local vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom or local array calculated by a compute with ID
f_ID = per-atom or local vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom or local array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name
- zero or more keyword/args pairs may be appended
- keyword = replace

replace args = vec1 vec2
vec1 = reduced value from this input vector will be replaced
vec2 = replace it with vec1[N] where N is index of max/min value from vec2

Examples:

compute 1 all reduce sum c_force
compute 1 all reduce/region subbox sum c_force
compute 2 all reduce min c_press2 f_ave v_myKE
compute 3 fluid reduce max c_index1 c_index2 c_dist replace 1 3 replace 2 3

Description:

Define a calculation that "reduces" one or more vector inputs into scalar values, one per listed input. The inputs can be per-atom or local quantities; they cannot be global quantities. Atom attributes are per-atom quantities, computes and fixes may generate any of the three kinds of quantities, and atom-style variables generate per-atom quantities. See the variable command and its special functions which can perform the same operations as the compute reduce command on global vectors.

The reduction operation is specified by the mode setting. The sum option adds the values in the vector into a global total. The min or max options find the minimum or maximum value across all vector values. The ave setting adds the vector values into a global total, then divides by the number of values in the vector.

Each listed input is operated on independently. For per-atom inputs, the group specified with this command means only atoms within the group contribute to the result. For per-atom inputs, if the compute reduce/region command is used, the atoms must also currently be within the region. Note that an input that produces per-atom
quantities may define its own group which affects the quantities it returns. For example, if a compute is used as an input which generates a per-atom vector, it will generate values of 0.0 for atoms that are not in the group specified for that compute.

Each listed input can be an atom attribute (position, velocity, force component) or can be the result of a compute or fix or the evaluation of an atom-style variable.

The atom attribute values (x,y,z,vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes can be used as inputs to this fix by using the compute property/atom command and then specifying an input value from that compute.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. Computes can generate per-atom or local quantities. See the individual compute doc page for details. If no bracketed integer is appended, the vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. Fixes can generate per-atom or local quantities. See the individual fix doc page for details. Note that some fixes only produce their values on certain timesteps, which must be compatible with when compute reduce references the values, else an error results. If no bracketed integer is appended, the vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the array calculated by the fix is used. Users can also write code for their own fix style and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. It must be an atom-style variable. Atom-style variables can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to reduce.

If the replace keyword is used, two indices vec1 and vec2 are specified, where each index ranges from 1 to the # of input values. The replace keyword can only be used if the mode is min or max. It works as follows. A min/max is computed as usual on the vec2 input vector. The index N of that value within vec2 is also stored. Then, instead of performing a min/max on the vec1 input vector, the stored index is used to select the Nth element of the vec1 vector.

Thus, for example, if you wish to use this compute to find the bond with maximum stretch, you can do it as follows:

```
compute 1 all property/local batom1 batom2
calculate 2 all bond/local dist
compute 3 all reduce max c_1[1] c_1[2] c_2 replace 1 3 replace 2 3
```

The first two input values in the compute reduce command are vectors with the IDs of the 2 atoms in each bond, using the compute property/local command. The last input value is bond distance, using the compute bond/local command. Instead of taking the max of the two atom ID vectors, which does not yield useful information in this context, the replace keywords will extract the atom IDs for the two atoms in the bond of maximum stretch. These atom IDs and the bond stretch will be printed with thermodynamic output.

If a single input is specified this compute produces a global scalar value. If multiple inputs are specified, this compute produces a global vector of values, the length of which is equal to the number of inputs specified.
As discussed below, for *sum* mode, the value(s) produced by this compute are all "extensive", meaning their value scales linearly with the number of atoms involved. If normalized values are desired, this compute can be accessed by the `thermo_style custom` command with `thermo_modify norm yes` set as an option. Or it can be accessed by a variable that divides by the appropriate atom count.

**Output info:**

This compute calculates a global scalar if a single input value is specified or a global vector of length *N* where *N* is the number of inputs, and which can be accessed by indices 1 to *N*. These values can be used by any command that uses global scalar or vector values from a compute as input. See Section howto 15 for an overview of LAMMPS output options.

All the scalar or vector values calculated by this compute are "intensive", except when the *sum* mode is used on per-atom or local vectors, in which case the calculated values are "extensive".

The scalar or vector values will be in whatever units the quantities being reduced are in.

**Restrictions:** none

**Related commands:**

compute, fix, variable

**Default:** none
compute slice command

Syntax:

compute ID group-ID slice Nstart Nstop Nskip input1 input2 ...

• ID, group-ID are documented in compute command
• slice = style name of this compute command
• Nstart = starting index within input vector(s)
• Nstop = stopping index within input vector(s)
• Nskip = extract every Nskip elements from input vector(s)
• input = c_ID, c_ID[N], f_ID, f_ID[N]

Example:

compute 1 all slice 1 100 10 c_msdmol[4]
compute 1 all slice 301 400 1 c_msdmol[4]

Description:

Define a calculation that "slices" one or more vector inputs into smaller vectors, one per listed input. The inputs can be global quantities; they cannot be per-atom or local quantities. Computes and fixes may generate any of the three kinds of quantities. Variables do not generate global vectors. The group specified with this command is ignored.

The values extracted from the input vector(s) are determined by the Nstart, Nstop, and Nskip parameters. The elements of an input vector of length N are indexed from 1 to N. Starting at element Nstart, every Mth element is extracted, where M = Nskip, until element Nstop is reached. The extracted quantities are stored as a vector, which is typically shorter than the input vector.

Each listed input is operated on independently to produce one output vector. Each listed input must be a global vector or column of a global array calculated by another compute or fix.

If an input value begins with "c_", a compute ID must follow which has been previously defined in the input script and which generates a global vector or array. See the individual compute doc page for details. If no bracketed integer is appended, the vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script and which generates a global vector or array. See the individual fix doc page for details. Note that some fixes only produce their values on certain timesteps, which must be compatible with when compute slice references the values, else an error results. If no bracketed integer is appended, the vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the array calculated by the fix is used. Users can also write code for their own fix style and add them to LAMMPS.

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If a single input is specified this compute produces a global vector, even if the length of the vector is 1. If multiple inputs are specified, then a global array of values is produced, with the number of columns equal to the number of inputs specified.

Output info:

This compute calculates a global vector if a single input value is specified or a global array with N columns where N is the number of inputs. The length of the vector or the number of rows in the array is equal to the number of values extracted from each input vector. These values can be used by any command that uses global vector or array values from a compute as input. See this section for an overview of LAMMPS output options.

The vector or array values calculated by this compute are simply copies of values generated by computes or fixes that are input vectors to this compute. If there is a single input vector of intensive and/or extensive values, then each value in the vector of values calculated by this compute will be "intensive" or "extensive", depending on the corresponding input value. If there are multiple input vectors, and all the values in them are intensive, then the array values calculated by this compute are "intensive". If there are multiple input vectors, and any value in them is extensive, then the array values calculated by this compute are "extensive".

The vector or array values will be in whatever units the input quantities are in.

Restrictions: none

Related commands:

compute, fix, compute reduce

Default: none
compute stress/atom command

**Syntax:**

```
compute ID group-ID stress/atom keyword ...
```

- ID, group-ID are documented in `compute` command
- `stress/atom` = style name of this compute command
- zero or more keywords may be appended
- `keyword` = `ke` or `pair` or `bond` or `angle` or `dihedral` or `improper` or `kspace` or `fix` or `virial`

**Examples:**

```
compute 1 mobile stress/atom
compute 1 all stress/atom pair bond
```

**Description:**

Define a computation that computes the symmetric per-atom stress tensor for each atom in a group. The tensor for each atom has 6 components and is stored as a 6-element vector in the following order: xx, yy, zz, xy, xz, yz. See the `compute pressure` command if you want the stress tensor (pressure) of the entire system.

The stress tensor for atom $I$ is given by the following formula, where $a$ and $b$ take on values x,y,z to generate the 6 components of the symmetric tensor:

$$ S_{ab} = - \left[ m v_a v_b + \frac{1}{2} \sum_{n=1}^{N_p} (r_{1a} F_{1b} + r_{2a} F_{2b}) + \frac{1}{2} \sum_{n=1}^{N_b} (r_{1a} F_{1b} + r_{2a} F_{2b}) + \frac{1}{3} \sum_{n=1}^{N_a} (r_{1a} F_{1b} + r_{2a} F_{2b} + r_{3a} F_{3b}) + \frac{1}{4} \sum_{n=1}^{N_d} (r_{1a} F_{1b} + r_{2a} F_{2b} + r_{3a} F_{3b} + r_{4a} F_{4b}) + \frac{1}{4} \sum_{n=1}^{N_i} (r_{1a} F_{1b} + r_{2a} F_{2b} + r_{3a} F_{3b} + r_{4a} F_{4b}) + Kspace(r_{i0}, F_{ib}) + \sum_{n=1}^{N_f} r_{ia} F_{ib} \right] $$

The first term is a kinetic energy contribution for atom $I$. The second term is a pairwise energy contribution where $n$ loops over the $N_p$ neighbors of atom $I$, $r1$ and $r2$ are the positions of the 2 atoms in the pairwise interaction, and $F1$ and $F2$ are the forces on the 2 atoms resulting from the pairwise interaction. The third term is a bond contribution of similar form for the $N_b$ bonds which atom $I$ is part of. There are similar terms for the $N_a$ angle, $N_d$ dihedral, and $N_i$ improper interactions atom $I$ is part of. There is also a term for the KSpace contribution from long-range Coulombic interactions, if defined. Finally, there is a term for the $N_f$ fixes that apply internal constraint forces to atom $I$. Currently, only the `fix shake` and `fix rigid` commands contribute to this term.

As the coefficients in the formula imply, a virial contribution produced by a small set of atoms (e.g. 4 atoms in a dihedral or 3 atoms in a Tersoff 3-body interaction) is assigned in equal portions to each atom in the set. E.g. 1/4 of the dihedral virial to each of the 4 atoms, or 1/3 of the fix virial due to SHAKE constraints applied to atoms in
a water molecule via the \texttt{fix shake} command.

If no extra keywords are listed, all of the terms in this formula are included in the per-atom stress tensor. If any extra keywords are listed, only those terms are summed to compute the tensor. The \textit{virial} keyword means include all terms except the kinetic energy \textit{ke}.

Note that the stress for each atom is due to its interaction with all other atoms in the simulation, not just with other atoms in the group.

The \texttt{dihedral_style charmm} style calculates pairwise interactions between 1-4 atoms. The virial contribution of these terms is included in the pair virial, not the dihedral virial.

The KSpace contribution is calculated using the method in \textit{(Heyes)} for the Ewald method and a related method for PPPM, as specified by the \texttt{kspace_style ppm} command. For PPPM, the calculation requires 6 extra FFTs each timestep that per-atom stress is calculated. Thus it can significantly increase the cost of the PPPM calculation if it is needed on a large fraction of the simulation timesteps.

Note that as defined in the formula, per-atom stress is the negative of the per-atom pressure tensor. It is also really a stress*volume formulation, meaning the computed quantity is in units of pressure*volume. It would need to be divided by a per-atom volume to have units of stress (pressure), but an individual atom's volume is not well defined or easy to compute in a deformed solid or a liquid. Thus, if the diagonal components of the per-atom stress tensor are summed for all atoms in the system and the sum is divided by \textit{dV}, where \textit{d} = dimension and \textit{V} is the volume of the system, the result should be \textit{-P}, where \textit{P} is the total pressure of the system.

These lines in an input script for a 3d system should yield that result. I.e. the last 2 columns of thermo output will be the same:

\begin{verbatim}
compute         peratom all stress/atom
thermo_style    custom step temp etotal press v_press
\end{verbatim}

\textbf{Output info:}

This compute calculates a per-atom array with 6 columns, which can be accessed by indices 1-6 by any command that uses per-atom values from a compute as input. See \texttt{Section\_howto 15} for an overview of LAMMPS output options.

The per-atom array values will be in pressure*volume units as discussed above.

\textbf{Restrictions:} none

\textbf{Related commands:}

\texttt{compute pe, compute pressure}

\textbf{Default:} none
compute temp command

compute temp/cuda command

Syntax:

compute ID group-ID temp

- ID, group-ID are documented in compute command
- temp = style name of this compute command

Examples:

compute 1 all temp
compute myTemp mobile temp

Description:

Define a computation that calculates the temperature of a group of atoms. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The temperature is calculated by the formula \( KE = \frac{dim}{2} N k T \), where \( KE \) = total kinetic energy of the group of atoms (sum of \( \frac{1}{2} m v^2 \)), \( dim = 2 \) or \( 3 \) = dimensionality of the simulation, \( N \) = number of atoms in the group, \( k \) = Boltzmann constant, and \( T \) = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that \( v^2 \) is replaced by \( vx*vy \) for the xy component, etc. The 6 components of the vector are ordered \( xx, yy, zz, xy, xz, yz \).

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the dynamic option of the compute_modify command if this is not the case.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the extra option of the compute_modify command.

A compute of this style with the ID of "thermo_temp" is created when LAMMPS starts up, as if this command were in the input script:

compute thermo_temp all temp

See the "thermo_style" command for more details.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual.
The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions: none

Related commands:

compute temp/partial, compute temp/region, compute pressure

Default: none
compute temp/asphere command

Syntax:

compute ID group-ID temp/asphere keyword value ...

- ID, group-ID are documented in compute command
- temp/asphere = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = bias or dof

bias value = bias-IDuniform or gaussian
  bias-ID = ID of a temperature compute that removes a velocity bias

dof value = all or rotate
  all = compute temperature of translational and rotational degrees of freedom
  rotate = compute temperature of just rotational degrees of freedom

Examples:

compute 1 all temp/asphere
compute myTemp mobile temp/asphere bias tempCOM
compute myTemp mobile temp/asphere dof rotate

Description:

Define a computation that calculates the temperature of a group of aspherical particles, including a contribution from both their translational and rotational kinetic energy. This differs from the usual compute temp command, which assumes point particles with only translational kinetic energy.

Only finite-size particles (aspherical or spherical) can be included in the group. For 3d finite-size particles, each has 6 degrees of freedom (3 translational, 3 rotational). For 2d finite-size particles, each has 3 degrees of freedom (2 translational, 1 rotational).

IMPORTANT NOTE: This choice for degrees of freedom (dof) assumes that all finite-size aspherical or spherical particles in your model will freely rotate, sampling all their rotational dof. It is possible to use a combination of interaction potentials and fixes that induce no torque or otherwise constrain some of all of your particles so that this is not the case. Then there are less dof and you should use the compute_modify extra command to adjust the dof accordingly.

For example, an aspherical particle with all three of its shape parameters the same is a sphere. If it does not rotate, then it should have 3 dof instead of 6 in 3d (or 2 instead of 3 in 2d). A uniaxial aspherical particle has two of its three shape parameters the same. If it does not rotate around the axis perpendicular to its circular cross section, then it should have 5 dof instead of 6 in 3d.

The translational kinetic energy is computed the same as is described by the compute temp command. The rotational kinetic energy is computed as 1/2 I w^2, where I is the inertia tensor for the aspherical particle and w is its angular velocity, which is computed from its angular momentum.

IMPORTANT NOTE: For 2d models, particles are treated as ellipsoids, not ellipses, meaning their moments of inertia will be the same as in 3d.
A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formula, except that \( v^2 \) and \( w^2 \) are replaced by \( vx*vy \) and \( wx*wy \) for the xy component, and the appropriate elements of the inertia tensor are used. The 6 components of the vector are ordered \( xx, yy, zz, xy, xz, yz \).

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the \textit{dynamic} option of the `compute_modify` command if this is not the case.

This compute subtracts out translational degrees-of-freedom due to fixes that constrain molecular motion, such as `fix shake` and `fix rigid`. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the `extra` option of the `compute_modify` command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

The keyword/value option pairs are used in the following ways.

For the \textit{bias} keyword, \textit{bias-ID} refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This allows compute temp/sphere to compute its thermal temperature after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a velocity profile. Thermostats that use this compute will work with this bias term. See the doc pages for individual computes that calculate a temperature and the doc pages for fixes that perform thermostatting for more details.

For the \textit{dof} keyword, a setting of \textit{all} calculates a temperature that includes both translational and rotational degrees of freedom. A setting of \textit{rotate} calculates a temperature that includes only rotational degrees of freedom.

\textbf{Output info:}

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature \textit{units}. The vector values will be in energy \textit{units}.

\textbf{Restrictions:}

This compute is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This compute requires that atoms store angular momementum and a quaternion as defined by the `atom_style ellipsoid` command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

\textbf{Related commands:}

`compute temp`
Default: none
compute temp/com command

Syntax:

compute ID group-ID temp/com

- ID, group-ID are documented in compute command
- temp/com = style name of this compute command

Examples:

compute 1 all temp/com
compute myTemp mobile temp/com

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out the center-of-mass velocity of the group. This is useful if the group is expected to have a non-zero net velocity for some reason. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

After the center-of-mass velocity has been subtracted from each atom, the temperature is calculated by the formula $KE = \frac{\text{dim}}{2} N k T$, where $KE = \text{total kinetic energy of the group of atoms (sum of } \frac{1}{2} m v^2\text{)}$, $\text{dim} = 2$ or $3 = \text{dimensionality of the simulation}$, $N = \text{number of atoms in the group}$, $k = \text{Boltzmann constant}$, and $T = \text{temperature}$.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that $v^2$ is replaced by $vx*vy$ for the xy component, etc. The 6 components of the vector are ordered $xx, yy, zz, xy, xz, yz$.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the dynamic option of the compute_modify command if this is not the case.

The removal of the center-of-mass velocity by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the extra option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Output info:
This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

**Restrictions:** none

**Related commands:**

compute temp

**Default:** none
compute temp/deform command

Syntax:

compute ID group-ID temp/deform

- ID, group-ID are documented in compute command
- temp/deform = style name of this compute command

Examples:

compute myTemp all temp/deform

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out a streaming velocity induced by the simulation box changing size and/or shape, for example in a non-equilibrium MD (NEMD) simulation. The size/shape change is induced by use of the fix deform command. A compute of this style is created by the fix nvt/sllod command to compute the thermal temperature of atoms for thermostatting purposes. A compute of this style can also be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The deformation fix changes the box size and/or shape over time, so each atom in the simulation box can be thought of as having a "streaming" velocity. For example, if the box is being sheared in x, relative to y, then atoms at the bottom of the box (low y) have a small x velocity, while atoms at the top of the box (hi y) have a large x velocity. This position-dependent streaming velocity is subtracted from each atom's actual velocity to yield a thermal velocity which is used to compute the temperature.

IMPORTANT NOTE: Fix deform has an option for remapping either atom coordinates or velocities to the changing simulation box. When using this compute in conjunction with a deforming box, fix deform should NOT remap atom positions, but rather should let atoms respond to the changing box by adjusting their own velocities (or let fix deform remap the atom velocities, see it's remap option). If fix deform does remap atom positions, then they appear to move with the box but their velocity is not changed, and thus they do NOT have the streaming velocity assumed by this compute. LAMMPS will warn you if fix deform is defined and its remap setting is not consistent with this compute.

After the streaming velocity has been subtracted from each atom, the temperature is calculated by the formula $KE = \frac{dim}{2} N k T$, where $KE =$ total kinetic energy of the group of atoms (sum of $\frac{1}{2} m v^2$), $dim = 2$ or $3 =$ dimensionality of the simulation, $N =$ number of atoms in the group, $k =$ Boltzmann constant, and $T =$ temperature. Note that $v$ in the kinetic energy formula is the atom's thermal velocity.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that $v^2$ is replaced by $vx*vy$ for the xy component, etc. The 6 components of the vector are ordered $xx, yy, zz, xy, xz, yz$.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the dynamic option of the compute_modify command if this is not the case.
The removal of the box deformation velocity component by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the extra option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions: none

Related commands:

compute temp/ramp, compute temp/profile, fix deform, fix nvt/sllod

Default: none
compute temp/deform/eff command

Syntax:

```plaintext
compute ID group-ID temp/deform/eff
```

- ID, group-ID are documented in `compute` command
- `temp/deform/eff` = style name of this compute command

Examples:

```plaintext
compute myTemp all temp/deform/eff
```

Description:

Define a computation that calculates the temperature of a group of nuclei and electrons in the electron force field model, after subtracting out a streaming velocity induced by the simulation box changing size and/or shape, for example in a non-equilibrium MD (NEMD) simulation. The size/shape change is induced by use of the `fix deform/eff` command. A compute of this style is created by the `fix nvt/sllod/eff` command to compute the thermal temperature of atoms for thermostatting purposes. A compute of this style can also be used by any command that computes a temperature, e.g. `thermo_modify`, `fix npt/eff`, etc.

The calculation performed by this compute is exactly like that described by the `compute temp/deform` command, except that the formula for the temperature includes the radial electron velocity contributions, as discussed by the `compute temp/eff` command. Note that only the translational degrees of freedom for each nuclei or electron are affected by the streaming velocity adjustment. The radial velocity component of the electrons is not affected.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

`compute temp/ramp`, `fix deform/eff`, `fix nvt/sllod/eff`

Default: none
compute temp/eff command

Syntax:

compute ID group-ID temp/eff

• ID, group-ID are documented in compute command
• temp/eff = style name of this compute command

Examples:

compute 1 all temp/eff
compute myTemp mobile temp/eff

Description:

Define a computation that calculates the temperature of a group of nuclei and electrons in the electron force field model. A compute of this style can be used by commands that compute a temperature, e.g. thermo_modify, fix npt/eff, etc.

The temperature is calculated by the formula \( KE = \text{dim}/2 \cdot N \cdot k \cdot T \), where \( KE \) = total kinetic energy of the group of atoms (sum of \( 1/2 \cdot m \cdot v^2 \) for nuclei and sum of \( 1/2 \cdot (m \cdot v^2 + 3/4 \cdot m \cdot s^2) \) for electrons, where \( s \) includes the radial electron velocity contributions), \( \text{dim} = 2 \) or \( 3 \) = dimensionality of the simulation, \( N \) = number of atoms (only total number of nuclei in the eFF (see the pair_eff command) in the group, \( k \) = Boltzmann constant, and \( T \) = temperature. This expression is summed over all nuclear and electronic degrees of freedom, essentially by setting the kinetic contribution to the heat capacity to \( 3/2k \) (where only nuclei contribute). This subtlety is valid for temperatures well below the Fermi temperature, which for densities two to five times the density of liquid H2 ranges from 86,000 to 170,000 K.

IMPORTANT NOTE: For eFF models, in order to override the default temperature reported by LAMMPS in the thermodynamic quantities reported via the thermo command, the user should apply a thermo_modify command, as shown in the following example:

compute effTemp all temp/eff
thermo_style custom step etotal pe ke temp press
thermo_modify temp effTemp

A 6-component kinetic energy tensor is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that \( v^2 \) is replaced by \( vx \cdot vy \) for the xy component, etc. For the eFF, again, the radial electronic velocities are also considered.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the dynamic option of the compute_modify command if this is not the case.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the extra option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.
Output info:

The scalar value calculated by this compute is "intensive", meaning it is independent of the number of atoms in the simulation. The vector values are "extensive", meaning they scale with the number of atoms in the simulation.

Restrictions:

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute temp/partial, compute temp/region, compute pressure

Default: none
**compute temp/partial command**

**compute temp/partial/cuda command**

Syntax:

```
compute ID group-ID temp/partial xflag yflag zflag
```

- ID, group-ID are documented in compute command
- temp/partial = style name of this compute command
- xflag, yflag, zflag = 0/1 for whether to exclude/include this dimension

Examples:

```
compute newT flow temp/partial 1 1 0
```

Description:

Define a computation that calculates the temperature of a group of atoms, after excluding one or more velocity components. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The temperature is calculated by the formula $KE = \frac{dim}{2} N k T$, where $KE =$ total kinetic energy of the group of atoms (sum of $1/2 m v^2$), $dim =$ dimensionality of the simulation, $N =$ number of atoms in the group, $k =$ Boltzmann constant, and $T =$ temperature. The calculation of $KE$ excludes the $x$, $y$, or $z$ dimensions if $xflag$, $yflag$, or $zflag = 0$. The dim parameter is adjusted to give the correct number of degrees of freedom.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the calculation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that $v^2$ is replaced by $vx*vy$ for the $xy$ component, etc. The 6 components of the vector are ordered $xx$, $yy$, $zz$, $xy$, $xz$, $yz$.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the dynamic option of the compute_modify command if this is not the case.

The removal of velocity components by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the extra option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.
Styles with a \textit{cuda} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section\_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \texttt{-suffix command-line switch} when you invoke LAMMPS, or you can use the \texttt{suffix} command in your input script.

See Section\_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

\textbf{Output info:}

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

\textbf{Restrictions:} none

\textbf{Related commands:}

compute temp, compute temp/region, compute pressure

\textbf{Default:} none
compute temp/profile command

Syntax:

compute ID group-ID temp/profile xflag yflag zflag binstyle args

- ID, group-ID are documented in compute command
- temp/profile = style name of this compute command
- xflag,yflag,zflag = 0/1 for whether to exclude/include this dimension
- binstyle = x or y or z or xy or yz or xz or xyz

\[ x \text{ arg} = N_x \]
\[ y \text{ arg} = N_y \]
\[ z \text{ arg} = N_z \]
\[ xy \text{ args} = N_x \ N_y \]
\[ yz \text{ args} = N_y \ N_z \]
\[ xz \text{ args} = N_x \ N_z \]
\[ xyz \text{ args} = N_x \ N_y \ N_z \]
\[ N_x, N_y, N_z = \text{number of velocity bins in x,y,z dimensions} \]

Examples:

```
compute myTemp flow temp/profile 1 1 1 x 10
compute myTemp flow temp/profile 0 1 1 xyz 20 20 20
```

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out a spatially-averaged velocity field, before computing the kinetic energy. This can be useful for thermostating a collection of atoms undergoing a complex flow, e.g. via a profile-unbiased thermostat (PUT) as described in (Evans). A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The `xflag`, `yflag`, `zflag` settings determine which components of average velocity are subtracted out.

The `binstyle` setting and its `N_x`, `N_y`, `N_z` arguments determine how bins are setup to perform spatial averaging. "Bins" can be 1d slabs, 2d pencils, or 3d bricks depending on which `binstyle` is used. The simulation box is partitioned conceptually into `N_x` by `N_y` by `N_z` bins. Depending on the `binstyle`, you may only specify one or two of these values; the others are effectively set to 1 (no binning in that dimension). For non-orthogonal (triclinic) simulation boxes, the bins are "tilted" slabs or pencils or bricks that are parallel to the tilted faces of the box. See the `region prism` command for a discussion of the geometry of tilted boxes in LAMMPS.

When a temperature is computed, the velocity for the set of atoms that are both in the compute group and in the same spatial bin is summed to compute an average velocity for the bin. This bias velocity is then subtracted from the velocities of individual atoms in the bin to yield a thermal velocity for each atom. Note that if there is only one atom in the bin, it's thermal velocity will thus be 0.0.

After the spatially-averaged velocity field has been subtracted from each atom, the temperature is calculated by the formula \( KE = \text{dim}/2 \ N \ k \ T \), where \( KE \) = total kinetic energy of the group of atoms (sum of 1/2 m v^2), \( \text{dim} = 2 \) or \( 3 \) = dimensionality of the simulation, \( N \) = number of atoms in the group, \( k \) = Boltzmann constant, and \( T \) = temperature.
A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that \( v^2 \) is replaced by \( vx \times vy \) for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the dynamic option of the compute_modify command if this is not the case.

The removal of the spatially-averaged velocity field by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the extra option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting. Using this compute in conjunction with a thermostatting fix, as explained there, will effectively implement a profile-unbiased thermostat (PUT), as described in (Evans).

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

You should not use too large a velocity-binning grid, especially in 3d. In the current implementation, the binned velocity averages are summed across all processors, so this will be inefficient if the grid is too large, and the operation is performed every timestep, as it will be for most thermostats.

Related commands:

compute temp, compute temp/ramp, compute temp/deform, compute pressure

Default:

The option default is units = lattice.

compute temp/ramp command

Syntax:

compute ID group-ID temp/ramp vdim vlo vhi dim clo chi keyword value ...

- ID, group-ID are documented in compute command
- temp/ramp = style name of this compute command
- vdim = vx or vy or vz
- vlo,vhi = subtract velocities between vlo and vhi (velocity units)
- dim = x or y or z
- clo,chi = lower and upper bound of domain to subtract from (distance units)
- zero or more keyword/value pairs may be appended
- keyword = units

units value = lattice or box

Examples:

compute 2nd middle temp/ramp vx 0 8 y 2 12 units lattice

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out an ramped velocity profile before computing the kinetic energy. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The meaning of the arguments for this command which define the velocity ramp are the same as for the velocity ramp command which was presumably used to impose the velocity.

After the ramp velocity has been subtracted from the specified dimension for each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

The units keyword determines the meaning of the distance units used for coordinates (c1,c2) and velocities (vlo,vhi). A box value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A lattice value means the distance units are in lattice spacings; e.g. velocity = lattice spacings / tau. The lattice command must have been previously used to define the lattice spacing.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the dynamic option of the compute_modify command if this is not the case.

The removal of the ramped velocity component by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs
thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the extra option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

**Output info:**

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

**Restrictions:** none

**Related commands:**

compute temp, compute temp/profile, compute temp/deform, compute pressure

**Default:**

The option default is units = lattice.
compute temp/region command

Syntax:

compute ID group-ID temp/region region-ID

- ID, group-ID are documented in compute command
- temp/region = style name of this compute command
- region-ID = ID of region to use for choosing atoms

Examples:

compute mine flow temp/region boundary

Description:

Define a computation that calculates the temperature of a group of atoms in a geometric region. This can be useful for thermostating one portion of the simulation box. E.g. a McDLT simulation where one side is cooled, and the other side is heated. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, etc.

Note that a region-style temperature can be used to thermostat with fix temp/rescale or fix langevin, but should probably not be used with Nose/Hoover style fixes (fix nvt, fix npt, or fix nph), if the degrees-of-freedom included in the computed T varies with time.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in both the group and region, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is compute each time the temperature is evaluated since it is assumed atoms can enter/leave the region. Thus there is no need to use the dynamic option of the compute_modify command for this compute style.

The removal of atoms outside the region by this fix is essentially computing the temperature after a "bias" has been removed, which in this case is the velocity of any atoms outside the region. If this compute is used with a fix command that performs thermostating then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin. This means any of the thermostatting fixes can operate on a geometric region of atoms, as defined by this compute.

Unlike other compute styles that calculate temperature, this compute does not subtract out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This is because those degrees of freedom (e.g. a constrained bond) can straddle the region boundary, and hence the concept is somewhat ill-defined. If needed the number of subtracted degrees-of-freedom can be set explicitly using the extra option of the compute_modify command.
See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

**Output info:**

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

**Restrictions:** none

**Related commands:**

compute temp, compute pressure

**Default:** none
**compute temp/region/eff command**

**Syntax:**

compute ID group-ID temp/region/eff region-ID

- ID, group-ID are documented in `compute` command
- temp/region/eff = style name of this compute command
- region-ID = ID of region to use for choosing atoms

**Examples:**

compute mine flow temp/region/eff boundary

**Description:**

Define a computation that calculates the temperature of a group of nuclei and electrons in the electron force field model, within a geometric region using the electron force field. A compute of this style can be used by commands that compute a temperature, e.g. `thermo_modify`.

The operation of this compute is exactly like that described by the `compute temp/region` command, except that the formula for the temperature itself includes the radial electron velocity contributions, as discussed by the `compute temp/eff` command.

**Output info:**

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

**Restrictions:**

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

`compute temp/region, compute temp/eff, compute pressure`

**Default:** none
compute temp/rotate command

Syntax:

compute ID group-ID temp/rotate

- ID, group-ID are documented in compute command
- temp/rotate = style name of this compute command

Examples:

compute Tbead bead temp/rotate

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out the center-of-mass velocity and angular velocity of the group. This is useful if the group is expected to have a non-zero net velocity and/or global rotation motion for some reason. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

After the center-of-mass velocity and angular velocity has been subtracted from each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the dynamic option of the compute modify command if this is not the case.

The removal of the center-of-mass velocity and angular velocity by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the extra option of the compute modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Output info:
This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

**Restrictions:**

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

compute temp

**Default:** none
**compute temp/sphere command**

**Syntax:**

```
compute ID group-ID temp/sphere keyword value ...
```

- ID, group-ID are documented in `compute` command
- `temp/sphere` = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = `bias` or `dof`

`bias` value = `bias-IDuniform` or `gaussian`
`bias-ID` = ID of a temperature compute that removes a velocity bias

`dof` value = `all` or `rotate`
  - `all` = compute temperature of translational and rotational degrees of freedom
  - `rotate` = compute temperature of just rotational degrees of freedom

**Examples:**

```
compute 1 all temp/sphere
compute myTemp mobile temp/sphere bias tempCOM
compute myTemp mobile temp/sphere dof rotate
```

**Description:**

Define a computation that calculates the temperature of a group of spherical particles, including a contribution from both their translational and rotational kinetic energy. This differs from the usual `compute temp` command, which assumes point particles with only translational kinetic energy.

Both point and finite-size particles can be included in the group. Point particles do not rotate, so they have only 3 translational degrees of freedom. For 3d spherical particles, each has 6 degrees of freedom (3 translational, 3 rotational). For 2d spherical particles, each has 3 degrees of freedom (2 translational, 1 rotational).

IMPORTANT NOTE: This choice for degrees of freedom (dof) assumes that all finite-size spherical particles in your model will freely rotate, sampling all their rotational dof. It is possible to use a combination of interaction potentials and fixes that induce no torque or otherwise constrain some of all of your particles so that this is not the case. Then there are less dof and you should use the `compute_modify extra` command to adjust the dof accordingly.

The translational kinetic energy is computed the same as is described by the `compute temp` command. The rotational kinetic energy is computed as \( \frac{1}{2} I w^2 \), where \( I \) is the moment of inertia for a sphere and \( w \) is the particle's angular velocity.

IMPORTANT NOTE: For 2d models, particles are treated as spheres, not disks, meaning their moment of inertia will be the same as in 3d.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formulas, except that \( v^2 \) and \( w^2 \) are replaced by \( vx*vy \) and \( wx*wy \) for the xy component. The 6 components of the vector are ordered \( xx, yy, zz, xy, xz, yz \).

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the `dynamic` option of the `compute_modify` command if this is not the case.
This compute subtracts out translational degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the extra option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

The keyword/value option pairs are used in the following ways.

For the bias keyword, bias-ID refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This allows compute temp/sphere to compute its thermal temperature after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a velocity profile. Thermostats that use this compute will work with this bias term. See the doc pages for individual computes that calculate a temperature and the doc pages for fixes that perform thermostatting for more details.

For the dof keyword, a setting of all calculates a temperature that includes both translational and rotational degrees of freedom. A setting of rotate calculates a temperature that includes only rotational degrees of freedom.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the atom_style sphere command.

All particles in the group must be finite-size spheres, or point particles with radius = 0.0.

Related commands:

compute temp, compute temp/asphere

Default:

The option defaults are no bias and dof = all.
compute ti command

Syntax:

compute ID group ti keyword args ...

- ID, group-ID are documented in compute command
- ti = style name of this compute command
- one or more attribute/arg pairs may be appended
- keyword = pair style (lj/cut, gauss, born, etc) or tail or kspace

Examples:

compute 1 all ti lj/cut v_lj v_dlj coul/long v_c v_dc kspace v_ks v_dks

Description:

Define a computation that calculates the derivative of the interaction potential with respect to lambda, the coupling parameter used in a thermodynamic integration. This derivative can be used to infer a free energy difference resulting from an alchemical simulation, as described in Eiike.

Typically this compute will be used in conjunction with the fix adapt command which can perform alchemical transformations by adjusting the strength of an interaction potential as a simulation runs, as defined by one or more pair_style or kspace_style commands. This scaling is done via a prefactor on the energy, forces, virial calculated by the pair or K-Space style. The prefactor is often a function of a lambda parameter which may be adjusted from 0 to 1 (or vice versa) over the course of a run. The time-dependent adjustment is what the fix adapt command does.

Assume that the unscaled energy of a pair_style or kspace_style is given by U. Then the scaled energy is

\[ Us = f(\lambda) U \]

where f() is some function of lambda. What this compute calculates is

\[ \frac{dUs}{d(\lambda)} = U \frac{df(\lambda)}{d\lambda} = Us \frac{df(\lambda)}{d\lambda} \]

which is the derivative of the system's scaled potential energy Us with respect to lambda.

To do this calculation, you provide two functions, as equal-style variables. The first is specified as v_name1, where name1 is the name of the variable, and is f(\lambda) in the notation above. The second is specified as v_name2, where name2 is the name of the variable, and is df(\lambda) / d\lambda in the notation above. I.e. it is the analytic derivative of f() with respect to lambda. Note that the name1 variable is also typically given as an
argument to the fix adapt command.

An alchemical simulation may use several pair potentials together, invoked via the pair_style hybrid or hybrid/overlay command. The total dU/dlambda for the overall system is calculated as the sum of each contributing term as listed by the keywords in the compute ti command. Individual pair potentials can be listed, which will be sub-styles in the hybrid case. You can also include a K-space term via the kspace keyword. You can also include a pairwise long-range tail correction to the energy via the tail keyword.

For each term you can specify a different (or the same) scale factor by the two variables that you list. Again, these will typically correspond to the scale factors applied to these various potentials and the K-Space contribution via the fix_adapt command.

More details about the exact functional forms for the computation of du/dl can be found in the paper by Eike.

Output info:

This compute calculates a global scalar, namely dU/dlambda. This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive".

The scalar value will be in energy units.

Restrictions: none

Related commands:

fix adapt

Default: none

create_atoms command

Syntax:

create_atoms type style args keyword values ...

- type = atom type (1-Ntypes) of atoms to create
- style = box or region or single or random
  - box args = none
  - region args = region-ID
    - region-ID = atoms will only be created if contained in the region
  - single args = x y z
    - x, y, z = coordinates of a single atom (distance units)
  - random args = N seed region-ID
    - N = number of atoms to create
    - seed = random # seed (positive integer)
    - region-ID = create atoms within this region, use NULL for entire simulation box
- zero or more keyword/value pairs may be appended
- keyword = basis or remap or units
  - basis values = M itype
    - M = which basis atom
    - itype = atom type (1-N) to assign to this basis atom
  - remap value = yes or no
  - units value = lattice or box
    - lattice = the geometry is defined in lattice units
    - box = the geometry is defined in simulation box units

Examples:

create_atoms 1 box
create_atoms 3 region regsphere basis 2 3
create_atoms 3 single 0 0 5

Description:

This command creates atoms on a lattice, or a single atom, or a random collection of atoms, as an alternative to reading in their coordinates explicitly via a read_data or read_restart command. A simulation box must already exist, which is typically created via the create_box command. Before using this command, a lattice must also be defined using the lattice command. The only exceptions are for the single style with units = box or the random style.

For the box style, the create_atoms command fills the entire simulation box with atoms on the lattice. If your simulation box is periodic, you should insure its size is a multiple of the lattice spacings, to avoid unwanted atom overlaps at the box boundaries. If your box is periodic and a multiple of the lattice spacing in a particular dimension, LAMMPS is careful to put exactly one atom at the boundary (on either side of the box), not zero or two.

For the region style, the geometric volume is filled that is inside the simulation box and is also consistent with the region volume. See the region command for details. Note that a region can be specified so that its "volume" is either inside or outside a geometric boundary. Also note that if your region is the same size as a periodic simulation box (in some dimension), LAMMPS does not implement the same logic as with the box style, to insure exactly one atom at the boundary. if this is what you desire, you should either use the box style, or tweak the
region size to get precisely the atoms you want.

For the *single* style, a single atom is added to the system at the specified coordinates. This can be useful for debugging purposes or to create a tiny system with a handful of atoms at specified positions.

For the *random* style, N atoms are added to the system at randomly generated coordinates, which can be useful for generating an amorphous system. The atoms are created one by one using the specified random number seed, resulting in the same set of atom coordinates, independent of how many processors are being used in the simulation. If the region-ID argument is specified as NULL, then the created atoms will be anywhere in the simulation box. If a region-ID is specified, a geometric volume is filled that is inside the simulation box and is also consistent with the region volume. See the region command for details. Note that a region can be specified so that its "volume" is either inside or outside a geometric boundary.

IMPORTANT NOTE: The atoms generated by the *random* style will typically be highly overlapped which will cause many interatomic potentials to compute large energies and forces. Thus you should either perform an energy minimization or run dynamics with fix nve/limit to equilibrate such a system, before running normal dynamics.

The *basis* keyword specifies an atom type that will be assigned to specific basis atoms as they are created. See the lattice command for specifics on how basis atoms are defined for the unit cell of the lattice. By default, all created atoms are assigned the argument *type* as their atom type.

The *remap* keyword only applies to the *single* style. If it is set to *yes*, then if the specified position is outside the simulation box, it will mapped back into the box, assuming the relevant dimensions are periodic. If it is set to *no*, no remapping is done and no atom is created if its position is outside the box.

The *units* keyword determines the meaning of the distance units used to specify the coordinates of the one atom created by the *single* style. A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings.

Note that this command adds atoms to those that already exist. By using the create_atoms command multiple times, multiple sets of atoms can be added to the simulation. For example, interleaving create_atoms with lattice commands specifying different orientations, grain boundaries can be created. By using the create_atoms command in conjunction with the delete_atoms command, reasonably complex geometries can be created. The create_atoms command can also be used to add atoms to a system previously read in from a data or restart file. In all these cases, care should be taken to insure that new atoms do not overlap existing atoms inappropriately. The delete_atoms command can be used to handle overlaps.

Atom IDs are assigned to created atoms in the following way. The collection of created atoms are assigned consecutive IDs that start immediately following the largest atom ID existing before the create_atoms command was invoked. When a simulation is performed on different numbers of processors, there is no guarantee a particular created atom will be assigned the same ID.

Aside from their ID, atom type, and xyz position, other properties of created atoms are set to default values, depending on which quantities are defined by the chosen atom style. See the atom style command for more details. See the set and velocity commands for info on how to change these values.

- charge = 0.0
- dipole moment magnitude = 0.0
- diameter = 1.0
- shape = 0.0 0.0 0.0
- density = 1.0

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• volume = 1.0
• velocity = 0.0 0.0 0.0
• angular velocity = 0.0 0.0 0.0
• angular momentum = 0.0 0.0 0.0
• quaternion = (1,0,0,0)
• bonds, angles, dihedrals, impropers = none

Note that the *sphere* atom style sets the default particle diameter to 1.0 as well as the density. This means the mass for the particle is not 1.0, but is \( \pi/6 \times \text{diameter}^3 = 0.5236 \).

Note that the *ellipsoid* atom style sets the default particle shape to (0.0 0.0 0.0) and the density to 1.0 which means it is a point particle, not an ellipsoid, and has a mass of 1.0.

Note that the *peri* style sets the default volume and density to 1.0 and thus also set the mass for the particle to 1.0.

The *set* command can be used to override many of these default settings.

**Restrictions:**

An *atom_style* must be previously defined to use this command.

**Related commands:**

lattice, region, create_box, read_data, read_restart

**Default:**

The default for the *basis* keyword is that all created atoms are assigned the argument *type* as their atom type. The default for *remap* = no and for *units* = lattice.
create_box command

Syntax:

create_box N region-ID

- N = # of atom types to use in this simulation
- region-ID = ID of region to use as simulation domain

Examples:

create_box 2 mybox

Description:

This command creates a simulation box based on the specified region. Thus a region command must first be used to define a geometric domain.

The argument N is the number of atom types that will be used in the simulation.

If the region is not of style prism, then LAMMPS encloses the region (block, sphere, etc) with an axis-aligned orthogonal bounding box which becomes the simulation domain.

If the region is of style prism, LAMMPS creates a non-orthogonal simulation domain shaped as a parallelepiped with triclinic symmetry. As defined by the region prism command, the parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by A = (xhi-xlo,0,0); B = (xy,yhi-ylo,0); C = (xz,yz,zhi-zlo). Xy,xz,yz can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped.

A prism region used with the create_box command must have tilt factors (xy,xz,yz) that do not skew the box more than half the distance of the parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all geometrically equivalent.

See Section_howto 12 of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

When a prism region is used, the simulation domain must be periodic in any dimensions with a non-zero tilt factor, as defined by the boundary command. I.e. if the xy tilt factor is non-zero, then both the x and y dimensions must be periodic. Similarly, x and z must be periodic if xz is non-zero and y and z must be periodic if yz is non-zero. Also note that if your simulation will tilt the box, e.g. via the fix deform command, the simulation box must be defined as triclinic, even if the tilt factors are initially 0.0.

IMPORTANT NOTE: If the system is non-periodic (in a dimension), then you should not make the lo/hi box dimensions (as defined in your region command) radically smaller/larger than the extent of the atoms you eventually plan to create, e.g. via the create_atoms command. For example, if your atoms extend from 0 to 50, you should not specify the box bounds as -10000 and 10000. This is because LAMMPS uses the specified box size to layout the 3d grid of processors. A huge (mostly empty) box will be sub-optimal for performance when
using "fixed" boundary conditions (see the boundary command). When using "shrink-wrap" boundary conditions (see the boundary command), a huge (mostly empty) box may cause a parallel simulation to lose atoms the first time that LAMMPS shrink-wraps the box around the atoms.

**Restrictions:**

An atom_style and region must have been previously defined to use this command.

**Related commands:**

create_atoms, region

**Default:** none
delete\_atoms command

Syntax:

\[\text{delete\_atoms} \text{ style} \text{ args} \text{ keyword} \text{ value} \ldots\]

- \text{style} = \text{group} \text{ or} \text{ region} \text{ or} \text{ overlap} \text{ or} \text{ porosity}

  \[
  \begin{align*}
  \text{group} & \quad \text{args} = \text{group-}ID \\
  \text{region} & \quad \text{args} = \text{region-}ID \\
  \text{overlap} & \quad \text{args} = \text{cutoff} \text{ group1-}ID \text{ group2-}ID \\
  \text{porosity} & \quad \text{args} = \text{region-}ID \text{ fraction} \text{ seed}
  \end{align*}
  \]

  - \text{cutoff} = \text{delete one atom from pairs of atoms within the cutoff (distance units)}
  - \text{group1-}ID = \text{one atom in pair must be in this group}
  - \text{group2-}ID = \text{other atom in pair must be in this group}

  - \text{fraction} = \text{delete this fraction of atoms}
  - \text{seed} = \text{random number seed (positive integer)}

- \text{zero or more keyword/value pairs may be appended}

- \text{keyword} = \text{compress}

  \[
  \text{compress} \quad \text{value} = \text{no} \text{ or} \text{ yes}
  \]

Examples:

- delete\_atoms group edge
- delete\_atoms region sphere compress no
- delete\_atoms overlap 0.3 all all
- delete\_atoms overlap 0.5 solvent colloid
- delete\_atoms porosity cube 0.1 482793

Description:

Delete the specified atoms. This command can be used to carve out voids from a block of material or to delete created atoms that are too close to each other (e.g. at a grain boundary).

For style group, all atoms belonging to the group are deleted.

For style region, all atoms in the region volume are deleted.

For style overlap pairs of atoms whose distance of separation is within the specified cutoff distance are searched for, and one of the 2 atoms is deleted. Only pairs where one of the two atoms is in the first group specified and the other atom is in the second group are considered. The atom that is in the first group is the one that is deleted.

Note that it is OK for the two group IDs to be the same (e.g. group all), or for some atoms to be members of both groups. In these cases, either atom in the pair may be deleted. Also note that if there are atoms which are members of both groups, the only guarantee is that at the end of the deletion operation, enough deletions will have occurred that no atom pairs within the cutoff will remain (subject to the group restriction). There is no guarantee that the minimum number of atoms will be deleted, or that the same atoms will be deleted when running on different numbers of processors.

For style porosity a specified fraction of atoms are deleted within the specified region. For example, if fraction is 0.1, then 10\% of the atoms will be deleted. The atoms to delete are chosen randomly. There is no guarantee that
the exact fraction of atoms will be deleted, or that the same atoms will be deleted when running on different numbers of processors.

If the compress keyword is set to yes, then after atoms are deleted, then atom IDs are re-assigned so that they run from 1 to the number of atoms in the system. This is not done for molecular systems (see the atom_style command), regardless of the compress setting, since it would foul up the bond connectivity that has already been assigned.

Restrictions:

The overlap styles requires inter-processor communication to acquire ghost atoms and build a neighbor list. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses set, etc). Since a neighbor list is used to find overlapping atom pairs, it also means that you must define a pair style with force cutoffs greater than or equal to the desired overlap cutoff between pairs of relevant atom types, even though the pair potential will not be evaluated.

If the special_bonds command is used with a setting of 0, then a pair of bonded atoms (1-2, 1-3, or 1-4) will not appear in the neighbor list, and thus will not be considered for deletion by the overlap styles. You probably don’t want to be deleting one atom in a bonded pair anyway.

Related commands:

create_atoms

Default:

The option defaults are compress = yes.
delete_bonds command

Syntax:

delete_bonds group-ID style args keyword ...

- group-ID = group ID
- style = multi or atom or bond or angle or dihedral or improper or stats

  multi args = none
  atom args = an atom type
  bond args = a bond type
  angle args = an angle type
  dihedral args = a dihedral type
  improper args = an improper type
  stats args = none

- zero or more keywords may be appended
- keyword = any or undo or remove or special

Examples:

delete_bonds frozen multi remove
delete_bonds all atom 4 special
delete_bonds all stats

Description:

Turn off (or on) molecular topology interactions, i.e. bonds, angles, dihedrals, impropers. This command is useful for deleting interactions that have been previously turned off by bond-breaking potentials. It is also useful for turning off topology interactions between frozen or rigid atoms. Pairwise interactions can be turned off via the neigh_modify exclude command. The fix shake command also effectively turns off certain bond and angle interactions.

For all styles, an interaction is only turned off (or on) if all the atoms involved are in the specified group. For style multi this is the only criterion applied - all types of bonds, angles, dihedrals, impropers in the group turned off.

For style atom, one or more of the atoms involved must also be of the specified type.

For style bond, only bonds are candidates for turn-off, and the bond must also be of the specified type. Styles angle, dihedral, and improper are treated similarly.

For style bond, you can set the type to 0 to delete bonds that have been previously broken by a bond-breaking potential (which sets the bond type to 0 when a bond is broken); e.g. see the bond_style quartic command.

For style stats no interactions are turned off (or on); the status of all interactions in the specified group is simply reported. This is useful for diagnostic purposes if bonds have been turned off by a bond-breaking potential during a previous run.

The default behavior of the delete_bonds command is to turn off interactions by toggling their type to a negative value, but not to permanently remove the interaction. E.g. a bond_type of 2 is set to -2. The neighbor list creation routines will not include such an interaction in their interaction lists. The default is also to not alter the list of 1-2, 1-3, 1-4 neighbors computed by the special_bonds command and used to weight pairwise force and energy.
calculations. This means that pairwise computations will proceed as if the bond (or angle, etc) were still turned on.

Several keywords can be appended to the argument list to alter the default behavior.

The *any* keyword changes the requirement that all atoms in the bond (angle, etc) must be in the specified group in order to turn-off the interaction. If any of the atoms in the interaction are in the specified group, it will be turned off (or on if the *undo* keyword is used).

The *undo* keyword inverts the delete_bonds command so that the specified bonds, angles, etc are turned on if they are currently turned off. This means a negative value is toggled to positive. Note that the fix shake command also sets bond and angle types negative, so this option should not be used on those interactions.

The *remove* keyword is invoked at the end of the delete_bonds operation. It causes turned-off bonds (angles, etc) to be removed from each atom's data structure and then adjusts the global bond (angle, etc) counts accordingly. Removal is a permanent change; removed bonds cannot be turned back on via the *undo* keyword. Removal does not alter the pairwise 1-2, 1-3, 1-4 weighting list.

The *special* keyword is invoked at the end of the delete_bonds operation, after (optional) removal. It re-computes the pairwise 1-2, 1-3, 1-4 weighting list. The weighting list computation treats turned-off bonds the same as turned-on. Thus, turned-off bonds must be removed if you wish to change the weighting list.

Note that the choice of *remove* and *special* options affects how 1-2, 1-3, 1-4 pairwise interactions will be computed across bonds that have been modified by the delete_bonds command.

**Restrictions:**

This command requires inter-processor communication to coordinate the deleting of bonds. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses set, etc).

If deleted bonds (angles, etc) are removed but the 1-2, 1-3, 1-4 weighting list is not recomputed, this can cause a later fix shake command to fail due to an atom's bonds being inconsistent with the weighting list. This should only happen if the group used in the fix command includes both atoms in the bond, in which case you probably should be recomputing the weighting list.

**Related commands:**

neigh_modify exclude, special_bonds, fix shake

**Default:** none
dielectric command

Syntax:

dielectric value

• value = dielectric constant

Examples:

dielectric 2.0

Description:

Set the dielectric constant for Coulombic interactions (pairwise and long-range) to this value. The constant is unitless, since it is used to reduce the strength of the interactions. The value is used in the denominator of the formulas for Coulombic interactions - e.g. a value of 4.0 reduces the Coulombic interactions to 25% of their default strength. See the pair_style command for more details.

Restrictions: none

Related commands:

pair_style

Default:

dielectric 1.0
**dihedral_style charmm command**

**dihedral_style charmm/omp command**

*Syntax:*

\[
\text{dihedral_style charmm}
\]

*Examples:*

\[
\text{dihedral_style charmm}
\]
\[
\text{dihedral_coeff 1 120.0 1 60 0.5}
\]

*Description:*

The *charmm* dihedral style uses the potential

\[
E = K [1 + \cos(n \phi - d)]
\]

See *(MacKerell)* for a description of the CHARMM force field. This dihedral style can also be used for the AMBER force field (see comment on weighting factors below). See *(Cornell)* for a description of the AMBER force field.

The following coefficients must be defined for each dihedral type via the *dihedral_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- n (integer >= 0)
- d (integer value of degrees)
- weighting factor (0.0 to 1.0)

The weighting factor is applied to pairwise interaction between the 1st and 4th atoms in the dihedral, which are computed by a CHARMM *pair_style* with epsilon and sigma values specified with a *pair_coeff* command. Note that this weighting factor is unrelated to the weighting factor specified by the *special_bonds* command which applies to all 1-4 interactions in the system.

For CHARMM force fields, the *special_bonds* 1-4 weighting factor should be set to 0.0. This is because the pair styles that contain "charmm" (e.g. *pair_style lj/charmm/coul/long*) define extra 1-4 interaction coefficients that are used by this dihedral style to compute those interactions explicitly. This means that if any of the weighting factors defined as dihedral coefficients (4th coeff above) are non-zero, then you must use a charmm pair style. Note that if you do not set the *special_bonds* 1-4 weighting factor to 0.0 (which is the default) then 1-4 interactions in dihedrals will be computed twice, once by the pair routine and once by the dihedral routine, which is probably not what you want.

For AMBER force fields, the *special_bonds* 1-4 weighting factor should be set to the AMBER defaults (1/2 and 5/6) and all the dihedral weighting factors (4th coeff above) should be set to 0.0. In this case, you can use any pair style you wish, since the dihedral does not need any 1-4 information.
Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**

This dihedral style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

**Related commands:**

dihedral_coeff

**Default:** none


dihedral_style class2 command

dihedral_style class2/omp command

Syntax:

dihedral_style class2

Examples:

dihedral_style class2
  dihedral_coeff 1 100 75 100 70 80 60
  dihedral_coeff * mbt 3.5945 0.1704 -0.5490 1.5228
  dihedral_coeff * ebt 0.3417 0.3264 -0.9036 0.1368 -0.8080 1.0119 1.1010
  dihedral_coeff 2 at 0.0 -0.1850 -0.7963 -2.0220 0.0 -0.3991 110.2453 105.1270
  dihedral_coeff * aat -13.5271 110.2453 105.1270
  dihedral_coeff * bb13 0.0 1.0119 1.1010

Description:

The class2 dihedral style uses the potential

\[
E = E_d + E_{mbt} + E_{ebt} + E_{at} + E_{aat} + E_{bb13}
\]

\[
E_d = \sum_{n=1}^{3} K_n \left[ 1 - \cos(n\phi - \phi_n) \right]
\]

\[
E_{mbt} = (r_{jk} - r_2) \left[ A_1 \cos(\phi) + A_2 \cos(2\phi) + A_3 \cos(3\phi) \right]
\]

\[
E_{ebt} = (r_{ij} - r_1) \left[ B_1 \cos(\phi) + B_2 \cos(2\phi) + B_3 \cos(3\phi) \right] +
          (r_{kl} - r_3) \left[ C_1 \cos(\phi) + C_2 \cos(2\phi) + C_3 \cos(3\phi) \right]
\]

\[
E_{at} = (\theta_{ijk} - \theta_1) \left[ D_1 \cos(\phi) + D_2 \cos(2\phi) + D_3 \cos(3\phi) \right] +
          (\theta_{jkl} - \theta_2) \left[ E_1 \cos(\phi) + E_2 \cos(2\phi) + E_3 \cos(3\phi) \right]
\]

\[
E_{aat} = M(\theta_{ijk} - \theta_1)(\theta_{jkl} - \theta_2) \cos(\phi)
\]

\[
E_{bb13} = N(r_{ij} - r_1)(r_{kl} - r_3)
\]

where \(E_d\) is the dihedral term, \(E_{mbt}\) is a middle-bond-torsion term, \(E_{ebt}\) is an end-bond-torsion term, \(E_{at}\) is an angle-torsion term, \(E_{aat}\) is an angle-angle-torsion term, and \(E_{bb13}\) is a bond-bond-13 term.

Theta1 and theta2 are equilibrium angles and \(r_1\) \(r_2\) \(r_3\) are equilibrium bond lengths.

See (Sun) for a description of the COMPASS class2 force field.
Coefficients for the Ed, Embt, Eebt, Eat, Eaat, and Ebb13 formulas must be defined for each dihedral type via the `dihedral_coeff` command as in the example above, or in the data file or restart files read by the `read_data` or `read_restart` commands.

These are the 6 coefficients for the Ed formula:

- K1 (energy)
- phi1 (degrees)
- K2 (energy)
- phi2 (degrees)
- K3 (energy)
- phi3 (degrees)

For the Embt formula, each line in a `dihedral_coeff` command in the input script lists 5 coefficients, the first of which is "mbt" to indicate they are MiddleBondTorsion coefficients. In a data file, these coefficients should be listed under a "MiddleBondTorsion Coeffs" heading and you must leave out the "mbt", i.e. only list 4 coefficients after the dihedral type.

- mbt
- A1 (energy/distance)
- A2 (energy/distance)
- A3 (energy/distance)
- r2 (distance)

For the Eebt formula, each line in a `dihedral_coeff` command in the input script lists 9 coefficients, the first of which is "ebt" to indicate they are EndBondTorsion coefficients. In a data file, these coefficients should be listed under a "EndBondTorsion Coeffs" heading and you must leave out the "ebt", i.e. only list 8 coefficients after the dihedral type.

- ebt
- B1 (energy/distance)
- B2 (energy/distance)
- B3 (energy/distance)
- C1 (energy/distance)
- C2 (energy/distance)
- C3 (energy/distance)
- r1 (distance)
- r3 (distance)

For the Eat formula, each line in a `dihedral_coeff` command in the input script lists 9 coefficients, the first of which is "at" to indicate they are AngleTorsion coefficients. In a data file, these coefficients should be listed under a "AngleTorsion Coeffs" heading and you must leave out the "at", i.e. only list 8 coefficients after the dihedral type.

- at
- D1 (energy/radian)
- D2 (energy/radian)
- D3 (energy/radian)
- E1 (energy/radian)
- E2 (energy/radian)
- E3 (energy/radian)
- theta1 (degrees)
• theta2 (degrees)

Theta1 and theta2 are specified in degrees, but LAMMPS converts them to radians internally; hence the units of D and E are in energy/radian.

For the Eaat formula, each line in a `dihedral_coeff` command in the input script lists 4 coefficients, the first of which is "aat" to indicate they are AngleAngleTorsion coefficients. In a data file, these coefficients should be listed under a "AngleAngleTorsion Coeffs" heading and you must leave out the "aat", i.e. only list 3 coefficients after the dihedral type.

• aat
• M (energy/radian^2)
• theta1 (degrees)
• theta2 (degrees)

Theta1 and theta2 are specified in degrees, but LAMMPS converts them to radians internally; hence the units of M are in energy/radian^2.

For the Ebb13 formula, each line in a `dihedral_coeff` command in the input script lists 4 coefficients, the first of which is "bb13" to indicate they are BondBond13 coefficients. In a data file, these coefficients should be listed under a "BondBond13 Coeffs" heading and you must leave out the "bb13", i.e. only list 3 coefficients after the dihedral type.

• bb13
• N (energy/distance^2)
• r1 (distance)
• r3 (distance)

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the CLASS2 package. See the Making LAMMPS section for more info on packages.

Related commands:

`dihedral_coeff`

Default: none
dihedral_coeff command

Syntax:

dihedral_coeff N args

- N = dihedral type (see asterisk form below)
- args = coefficients for one or more dihedral types

Examples:

dihedral_coeff 1 80.0 1 3
dihedral_coeff * 80.0 1 3 0.5
dihedral_coeff 2* 80.0 1 3 0.5

Description:

Specify the dihedral force field coefficients for one or more dihedral types. The number and meaning of the coefficients depends on the dihedral style. Dihedral coefficients can also be set in the data file read by the read_data command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple dihedral types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of dihedral types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using a dihedral_coeff command can override a previous setting for the same dihedral type. For example, these commands set the coeffs for all dihedral types, then overwrite the coeffs for just dihedral type 2:

dihedral_coeff * 80.0 1 3
dihedral_coeff 2 200.0 1 3

da line in a data file that specifies dihedral coefficients uses the exact same format as the arguments of the dihedral_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Dihedral Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

1 80.0 1 3

The dihedral_style class2 is an exception to this rule, in that an additional argument is used in the input script to allow specification of the cross-term coefficients. See its doc page for details.

IMPORTANT NOTE: When comparing the formulas and coefficients for various LAMMPS dihedral styles with dihedral equations defined by other force fields, note that some force field implementations divide/multiply the energy prefactor $K$ by the multiple number of torsions that contain the J-K bond in an I-J-K-L torsion. LAMMPS does not do this, i.e. the listed dihedral equation applies to each individual dihedral. Thus you need to define $K$ appropriately to account for this difference if necessary.

Here is an alphabetic list of dihedral styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated dihedral_coeff command.
Note that there are also additional dihedral styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the dihedral section of this page.

- \texttt{dihedral_style none} - turn off dihedral interactions
- \texttt{dihedral_style hybrid} - define multiple styles of dihedral interactions
- \texttt{dihedral_style charmm} - CHARMM dihedral
- \texttt{dihedral_style class2} - COMPASS (class 2) dihedral
- \texttt{dihedral_style harmonic} - harmonic dihedral
- \texttt{dihedral_style helix} - helix dihedral
- \texttt{dihedral_style multi/harmonic} - multi-harmonic dihedral
- \texttt{dihedral_style opls} - OPLS dihedral

\textbf{Restrictions:}

This command must come after the simulation box is defined by a \texttt{read_data}, \texttt{read_restart}, or \texttt{create_box} command.

A dihedral style must be defined before any dihedral coefficients are set, either in the input script or in a data file.

\textbf{Related commands:}

\texttt{dihedral_style}

\textbf{Default:} none
dihedral_style cosine/shift/exp command

dihedral_style cosine/shift/exp/omp command

Syntax:

```
dihedral_style cosine/shift/exp
```

Examples:

```
dihedral_style cosine/shift/exp
dihedral_coeff 1 10.0 45.0 2.0
```

Description:

The \textit{cosine/shift/exp} dihedral style uses the potential

\[
E = -U_{\text{min}} \frac{e^{-a U(\theta, \theta_0)}}{e^a - 1} - 1
\]

with \(U(\theta, \theta_0) = -0.5 (1 + \cos(\theta - \theta_0))\)

where \(U_{\text{min}}, \theta, \text{and } a\) are defined for each dihedral type.

The potential is bounded between \([-U_{\text{min}}:0]\) and the minimum is located at the angle \(\theta_0\). The \(a\) parameter can be both positive or negative and is used to control the spring constant at the equilibrium.

The spring constant is given by k\(=a \exp(a) U_{\text{min}}/[2 (\exp(a)-1)]\). For \(a>3\) k\(=a/2\) to better than 5% relative error. For negative values of the \(a\) parameter, the spring constant is essentially zero, and anharmonic terms takes over. The potential is furthermore well behaved in the limit \(a>0\), where it has been implemented to linear order in \(a\) for \(a < 0.001\).

The following coefficients must be defined for each dihedral type via the \texttt{dihedral_coeff} command as in the example above, or in the data file or restart files read by the \texttt{read_data} or \texttt{read_restart} commands:

- \texttt{umin} (energy)
- \texttt{theta} (angle)
- \texttt{A} (real number)

Styles with a \textit{cuda}, \textit{gpu}, \textit{omp}, or \textit{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section \texttt{accelerate} of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \texttt{-suffix} command-line switch when you invoke LAMMPS, or you can use the \texttt{suffix} command in your input
See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**

This dihedral style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

**Related commands:**

dihedral_coeff, angle_cosineshiftexp

**Default:** none
dihedral_style harmonic command

dihedral_style harmonic/omp command

Syntax:

dihedral_style harmonic

Examples:

dihedral_style harmonic
dihedral_coeff 1 80.0 1 2

Description:

The *harmonic* dihedral style uses the potential

\[ E = K \left[ 1 + d \cos(n \phi) \right] \]

The following coefficients must be defined for each dihedral type via the `dihedral_coeff` command as in the example above, or in the data file or restart files read by the `read_data` or `read_restart` commands:

- K (energy)
- d (+1 or -1)
- n (integer >= 0)

IMPORTANT NOTE: Here are important points to take note of when defining LAMMPS dihedral coefficients for the harmonic style, so that they are compatible with how harmonic dihedrals are defined by other force fields:

- The LAMMPS convention is that the trans position = 180 degrees, while in some force fields trans = 0 degrees.
- Some force fields reverse the sign convention on d.
- Some force fields let n be positive or negative which corresponds to d = 1 or -1 for the harmonic style.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.
Restrictions:

This dihedral style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none
**dihedral_style helix command**

**dihedral_style helix/omp command**

**Syntax:**

```
dihedral_style helix
```

**Examples:**

```
dihedral_style helix
dihedral_coeff 1 80.0 100.0 40.0
```

**Description:**

The *helix* dihedral style uses the potential

\[
E = A[1 - \cos(\theta)] + B[1 + \cos(3\theta)] + C[1 + \cos(\theta + \frac{\pi}{4})]
\]

This coarse-grain dihedral potential is described in (Guo). For dihedral angles in the helical region, the energy function is represented by a standard potential consisting of three minima, one corresponding to the trans (t) state and the other to gauche states (g+ and g-). The paper describes how the A,B,C parameters are chosen so as to balance secondary (largely driven by local interactions) and tertiary structure (driven by long-range interactions).

The following coefficients must be defined for each dihedral type via the `dihedral_coeff` command as in the example above, or in the data file or restart files read by the `read_data` or `read_restart` commands:

- A (energy)
- B (energy)
- C (energy)

Styles with a *cuda*, *gpu*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**
This dihedral style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

**Related commands:**

`dihedral_coeff`

**Default:** none

---

dihedral_style hybrid command

Syntax:

dihedral_style hybrid style1 style2 ...

- style1,style2 = list of one or more dihedral styles

Examples:

dihedral_style hybrid harmonic helix
dihedral_coeff 1 harmonic 6.0 1 3
dihedral_coeff 2* helix 10 10 10

Description:

The hybrid style enables the use of multiple dihedral styles in one simulation. A dihedral style is assigned to each dihedral type. For example, dihedrals in a polymer flow (of dihedral type 1) could be computed with a harmonic potential and dihedrals in the wall boundary (of dihedral type 2) could be computed with a helix potential. The assignment of dihedral type to style is made via the dihedral_coeff command or in the data file.

In the dihedral_coeff commands, the name of a dihedral style must be added after the dihedral type, with the remaining coefficients being those appropriate to that style. In the example above, the 2 dihedral_coeff commands set dihedrals of dihedral type 1 to be computed with a harmonic potential with coefficients 6.0, 1, 3 for K, d, n. All other dihedral types (2-N) are computed with a helix potential with coefficients 10, 10, 10 for A, B, C.

If dihedral coefficients are specified in the data file read via the read_data command, then the same rule applies. E.g. "harmonic" or "helix", must be added after the dihedral type, for each line in the "Dihedral Coeffs" section, e.g.

Dihedral Coeffs

1 harmonic 6.0 1 3
2 helix 10 10 10
...

If class2 is one of the dihedral hybrid styles, the same rule holds for specifying additional AngleTorsion (and EndBondTorsion, etc) coefficients either via the input script or in the data file. I.e. class2 must be added to each line after the dihedral type. For lines in the AngleTorsion (or EndBondTorsion, etc) section of the data file for dihedral types that are not class2, you must use an dihedral style of skip as a placeholder, e.g.

AngleTorsion Coeffs

1 skip
2 class2 1.0 1.0 1.0 3.0 3.0 3.0 30.0 50.0
...

Note that it is not necessary to use the dihedral style skip in the input script, since AngleTorsion (or EndBondTorsion, etc) coefficients need not be specified at all for dihedral types that are not class2.

A dihedral style of none with no additional coefficients can be used in place of a dihedral style, either in a input script dihedral_coeff command or in the data file, if you desire to turn off interactions for specific dihedral types.
Restrictions:

This dihedral style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Unlike other dihedral styles, the hybrid dihedral style does not store dihedral coefficient info for individual sub-styles in a binary restart files. Thus when restarting a simulation from a restart file, you need to re-specify dihedral_coeff commands.

Related commands:

- dihedral_coeff

Default: none
dihedral_style multi/harmonic command

dihedral_style multi/harmonic/omp command

Syntax:

dihedral_style multi/harmonic

Examples:

dihedral_style multi/harmonic
dihedral_coeff 1 20 20 20 20 20

Description:

The multi/harmonic dihedral style uses the potential

\[ E = \sum_{n=1,5} A_n \cos^{n-1}(\phi) \]

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- A1 (energy)
- A2 (energy)
- A3 (energy)
- A4 (energy)
- A5 (energy)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.
Related commands:
dihedral_coeff

Default: none
dihedral_style none command

Syntax:

dihedral_style none

Examples:

dihedral_style none

Description:

Using an dihedral style of none means dihedral forces are not computed, even if quadruplets of dihedral atoms were listed in the data file read by the read_data command.

Restrictions: none

Related commands: none

Default: none
dihedral_style opls command

dihedral_style opls/omp command

Syntax:

dihedral_style opls

Examples:

dihedral_style opls
dihedral_coeff 1 90.0 90.0 90.0 70.0

Description:

The opls dihedral style uses the potential

\[ E = \frac{1}{2}K_1[1 + \cos(\phi)] + \frac{1}{2}K_2[1 - \cos(2\phi)] + \frac{1}{2}K_3[1 + \cos(3\phi)] + \frac{1}{2}K_4[1 - \cos(4\phi)] \]

Note that the usual 1/2 factor is not included in the K values.

This dihedral potential is used in the OPLS force field and is described in (Watkins).

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K1 (energy)
- K2 (energy)
- K3 (energy)
- K4 (energy)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:
This dihedral style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

dihedral_style command

Syntax:

dihedral_style style

• style = none or hybrid or charmm or class2 or harmonic or helix or multi/harmonic or opls

Examples:

dihedral_style harmonic
dihedral_style multi/harmonic
dihedral_style hybrid harmonic charmm

Description:

Set the formula(s) LAMMPS uses to compute dihedral interactions between quadruplets of atoms, which remain in force for the duration of the simulation. The list of dihedral quadruplets is read in by a read_data or read_restart command from a data or restart file.

Hybrid models where dihedrals are computed using different dihedral potentials can be setup using the hybrid dihedral style.

The coefficients associated with a dihedral style can be specified in a data or restart file or via the dihedral_coeff command.

All dihedral potentials store their coefficient data in binary restart files which means dihedral_style and dihedral_coeff commands do not need to be re-specified in an input script that restarts a simulation. See the read_restart command for details on how to do this. The one exception is that dihedral_style hybrid only stores the list of sub-styles in the restart file; dihedral coefficients need to be re-specified.

IMPORTANT NOTE: When both a dihedral and pair style is defined, the special_bonds command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between 4 bonded atoms.

In the formulas listed for each dihedral style, phi is the torsional angle defined by the quadruplet of atoms. This angle has a sign convention as shown in this diagram:

where the I,J,K,L ordering of the 4 atoms that define the dihedral is from left to right.
This sign convention effects several of the dihedral styles listed below (e.g. charmm, helix) in the sense that the energy formula depends on the sign of phi, which may be reflected in the value of the coefficients you specify.

IMPORTANT NOTE: When comparing the formulas and coefficients for various LAMMPS dihedral styles with dihedral equations defined by other force fields, note that some force field implementations divide/multiply the energy prefactor $K$ by the multiple number of torsions that contain the J-K bond in an I-J-K-L torsion. LAMMPS does not do this, i.e. the listed dihedral equation applies to each individual dihedral. Thus you need to define $K$ appropriately via the `dihedral_coeff` command to account for this difference if necessary.

Here is an alphabetic list of dihedral styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated `dihedral_coeff` command.

Note that there are also additional dihedral styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the dihedral section of this page.

- `dihedral_style none` - turn off dihedral interactions
- `dihedral_style hybrid` - define multiple styles of dihedral interactions
- `dihedral_style charmm` - CHARMM dihedral
- `dihedral_style class2` - COMPASS (class 2) dihedral
- `dihedral_style harmonic` - harmonic dihedral
- `dihedral_style helix` - helix dihedral
- `dihedral_style multi/harmonic` - multi-harmonic dihedral
- `dihedral_style opls` - OPLS dihedral

Restrictions:

Dihedral styles can only be set for atom styles that allow dihedrals to be defined.

Most dihedral styles are part of the MOLECULAR package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual dihedral potentials tell if it is part of a package.

Related commands:

- `dihedral_coeff`

Default:

- `dihedral_style none`
**dihedral_style table command**

**dihedral_style table/omp command**

**Syntax:**

`dihedral_style table style Ntable`

- `style = linear or spline` = method of interpolation
- `Ntable` = size of the internal lookup table

**Examples:**

`dihedral_style table spline 400`
`dihedral_style table linear 1000`
`dihedral_coeff 1 file.table DIH_TABLE1`
`dihedral_coeff 2 file.table DIH_TABLE2`

**Description:**

The `table` dihedral style creates interpolation tables of length `Ntable` from dihedral potential and derivative values listed in a file(s) as a function of the dihedral angle "phi". The files are read by the `dihedral_coeff` command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and derivative values at each of `Ntable` dihedral angles. During a simulation, these tables are used to interpolate energy and force values on individual atoms as needed. The interpolation is done in one of 2 styles: linear or spline.

For the `linear` style, the dihedral angle (phi) is used to find 2 surrounding table values from which an energy or its derivative is computed by linear interpolation.

For the `spline` style, cubic spline coefficients are computed and stored at each of the `Ntable` evenly-spaced values in the interpolated table. For a given dihedral angle (phi), the appropriate coefficients are chosen from this list, and a cubic polynomial is used to compute the energy and the derivative at this angle.

The following coefficients must be defined for each dihedral type via the `dihedral_coeff` command as in the example above.

- `filename`
- `keyword`

The filename specifies a file containing tabulated energy and derivative values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments). It can begin with one or more comment or blank lines.

```
# Table of the potential and its negative derivative
DIH_TABLE1                   (keyword is the first text on line)
N 30 DEGREES                 (N, NOF, DEGREES, RADIANS, CHECKU/F)
```
A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the dihedral_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the angle value, the 3rd value is the energy (in energy units), and the 4th is -dE/d(\phi) also in energy units). The 3rd term is the energy of the 4-atom configuration for the specified angle. The 4th term (when present) is the negative derivative of the energy with respect to the angle (in degrees, or radians depending on whether the user selected DEGREES or RADIANS). Thus the units of the last term are still energy, not force. The dihedral angle values must increase from one line to the next.

Dihedral table splines are cyclic. There is no discontinuity at 180 degrees (or at any other angle). Although in the examples above, the angles range from -180 to 180 degrees, in general, the first angle in the list can have any value (positive, zero, or negative). However the range of angles represented in the table must be strictly less than 360 degrees (2\pi radians) to avoid angle overlap. (You may not supply entries in the table for both 180 and -180, for example.) If the user's table covers only a narrow range of dihedral angles, strange numerical behavior can occur in the large remaining gap.

Parameters:

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the N specified in the dihedral_style table command. Let Ntable be the number of table entries requested dihedral_style command, and let Nfile be the parameter following "N" in the tabulated file ("30" in the sparse example above). What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and derivative values at Ntable different points (which are evenly spaced over a 360 degree range, even if the angles in the file are not). The resulting tables of length Ntable are then used as described above, when computing energy and force for individual dihedral angles and their atoms. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively nonpreliminary interpolation), you should set Ntable = Nfile. To insure the nodal points in the user's file are aligned with the interpolated table entries, the angles in the table should be integer multiples of 360/Ntable degrees, or 2*\pi/Ntable radians (depending on your choice of angle units).

The optional "NOF" keyword allows the user to omit the forces (negative energy derivatives) from the table file (normally located in the 4th column). In their place, forces will be calculated automatically by differentiating the
potential energy function indicated by the 3rd column of the table (using either linear or spline interpolation).

The optional "DEGREES" keyword allows the user to specify angles in degrees instead of radians (default).

The optional "RADIANS" keyword allows the user to specify angles in radians instead of degrees. (Note: This changes the way the forces are scaled in the 4th column of the data file.)

The optional "CHECKU" keyword is followed by a filename. This allows the user to save all of the the Ntable different entries in the interpolated energy table to a file to make sure that the interpolated function agrees with the user's expectations. (Note: You can temporarily increase the Ntable parameter to a high value for this purpose. "Ntable" is explained above.)

The optional "CHECKF" keyword is analogous to the "CHECKU" keyword. It is followed by a filename, and it allows the user to check the interpolated force table. This option is available even if the user selected the "NOF" option.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none
dimension command

Syntax:

dimension N

- N = 2 or 3

Examples:

dimension 2

Description:

Set the dimensionality of the simulation. By default LAMMPS runs 3d simulations. To run a 2d simulation, this command should be used prior to setting up a simulation box via the create_box or read_data commands. Restart files also store this setting.

See the discussion in Section_howto for additional instructions on how to run 2d simulations.

IMPORTANT NOTE: Some models in LAMMPS treat particles as extended spheres or ellipsoids, as opposed to point particles. In 2d, the particles will still be spheres or ellipsoids, not circular disks or ellipses, meaning their moment of inertia will be the same as in 3d.

Restrictions:

This command must be used before the simulation box is defined by a read_data or create_box command.

Related commands:

fix enforce2d

Default:

dimension 3
displace_atoms command

Syntax:

displace_atoms group-ID style args keyword value ...

- group-ID = ID of group of atoms to displace
- style = move or ramp or random

move args = delx dely delz
delx, dely, delz = distance to displace in each dimension (distance units)
ramp args = ddim dlo dhi dim clo chi
ddim = x or y or z
dlo, dhi = displacement distance between dlo and dhi (distance units)
dim = x or y or z
clo, chi = lower and upper bound of domain to displace (distance units)
random args = dx dy dz seed
dx, dy, dz = random displacement magnitude in each dimension (distance units)
seed = random # seed (positive integer)

- zero or more keyword/value pairs may be appended

keyword = units
value = box or lattice

Examples:

displace_atoms top move 0 -5 0 units box
displace_atoms flow ramp x 0.0 5.0 y 2.0 20.5

Description:

Displace a group of atoms. This can be used to move atoms a large distance before beginning a simulation or to randomize atoms initially on a lattice. For example, in a shear simulation, an initial strain can be imposed on the system. Or two groups of atoms can be brought into closer proximity.

The move style displaces the group of atoms by the specified 3d distance.

The ramp style displaces atoms a variable amount in one dimension depending on the atom's coordinate in a (possibly) different dimension. For example, the second example command displaces atoms in the x-direction an amount between 0.0 and 5.0 distance units. Each atom's displacement depends on the fractional distance its y coordinate is between 2.0 and 20.5. Atoms with y-coordinates outside those bounds will be moved the minimum (0.0) or maximum (5.0) amount.

The random style independently moves each atom in the group by a random displacement, uniformly sampled from a value between -dx and +dx in the x dimension, and similarly for y and z. Random numbers are used in such a way that the displacement of a particular atom is the same, regardless of how many processors are being used.

Distance units for displacement are determined by the setting of box or lattice for the units keyword. Box means distance units as defined by the units command - e.g. Angstroms for real units. Lattice means distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing.
IMPORTANT NOTE: Care should be taken not to move atoms on top of other atoms. After the move, atoms are remapped into the periodic simulation box if needed, and any shrink-wrap boundary conditions (see the boundary command) are enforced which may change the box size. Other than this effect, this command does not change the size or shape of the simulation box. See the change_box command if that effect is desired.

IMPORTANT NOTE: Atoms can be moved arbitrarily long distances by this command. If the simulation box is non-periodic and shrink-wrapped (see the boundary command), this can change its size or shape. This is not a problem, except that the mapping of processors to the simulation box is not changed by this command from its initial 3d configuration; see the processors command. Thus, if the box size/shape changes dramatically, the mapping of processors to the simulation box may not end up as optimal as the initial mapping attempted to be.

Restrictions: none

Related commands:
lattice, change_box

Default:
The option defaults are units = lattice.
dump command

dump image command

dump molfile command

Syntax:

dump ID group-ID style N file args

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be dumped
- style = atom or cfg or dcd or xtc or xyz or image or molfile or local or custom
- N = dump every this many timesteps
- file = name of file to write dump info to
- args = list of arguments for a particular style

atom args = none
cfg args = same as custom args, see below
dcd args = none
xtc args = none
xyz args = none

image args = discussed on dump image doc page

molfile args = discussed on dump molfile doc page

local args = list of local attributes
  possible attributes = index, c_ID, c_ID[N], f_ID, f_ID[N]
  index = enumeration of local values
  c_ID = local vector calculated by a compute with ID
  c_ID[N] = Nth column of local array calculated by a compute with ID
  f_ID = local vector calculated by a fix with ID
  f_ID[N] = Nth column of local array calculated by a fix with ID

custom args = list of atom attributes
  possible attributes = id, mol, type, element, mass,
  x, y, z, xs, ys, zs, xu, yu, zu,
  xsu, ysu, zsu, ix, iy, iz,
  vx, vy, vz, fx, fy, fz,
  q, mux, muy, muz, mu,
  radius, diameter, omega_x, omega_y, omega_z,
  angmom_x, angmom_y, angmom_z, tqx, tqy, tqz,
  spin, eradius, eravel, erforce,
  c_ID, c_ID[N], f_ID, f_ID[N], v_name

id = atom ID
mol = molecule ID
type = atom type
element = name of atom element, as defined by dump_modify command
mass = atom mass
x,y,z = unscaled atom coordinates
xs,ys,zs = scaled atom coordinates
xu,yu,zu = unwrapped atom coordinates
xsu,ysu,zsu = scaled unwrapped atom coordinates
ix,iy,iz = box image that the atom is in
vx, vy, vz = atom velocities
fx, fy, fz = forces on atoms
q = atom charge
mux, muy, muz = orientation of dipole moment of atom
mu = magnitude of dipole moment of atom
radius, diameter = radius, diameter of spherical particle
omegax, omegay, omegaz = angular velocity of extended particle
angmomx, angmomy, angmomz = angular momentum of extended particle
tqx, tqy, tqz = torque on extended particles
spin = electron spin
eradius = electron radius
ervel = electron radial velocity
erforce = electron radial force
c_ID = per-atom vector calculated by a compute with ID
c_ID[N] = Nth column of per-atom array calculated by a compute with ID
f_ID = per-atom vector calculated by a fix with ID
f_ID[N] = Nth column of per-atom array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name

Examples:

dump myDump all atom 100 dump.atom
dump 2 subgroup atom 50 dump.run.bin
dump 4a all custom 100 dump.myforce.* id type x y vx fx
dump 4b flow custom 100 dump.% myforce id type c_myF[3] v_ke
dump 2 inner cfg 10 dump.snap.*.cfg id type xs ys zs vx vy vz
dump snap all cfg 100 dump.config.*.cfg id type xs ys zs id type c_Stress2
dump 1 all xtc 1000 file.xtc
dump e_data all custom 100 dump.eff id type x y z spin eradius fx fy fz eforce

Description:

Dump a snapshot of atom quantities to one or more files every N timesteps in one of several styles. The image style is the exception; it creates a JPG or PPM image file of the atom configuration every N timesteps, as discussed on the dump image doc page. The timesteps on which dump output is written can also be controlled by a variable. See the dump_modify every command.

Only information for atoms in the specified group is dumped. The dump_modify thresh and region commands can also alter what atoms are included. Not all styles support all these options; see details below.

As described below, the filename determines the kind of output (text or binary or gzipped, one big file or one per timestep, one big file or one per processor).

IMPORTANT NOTE: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom written to a dump file may be slightly outside the simulation box.

IMPORTANT NOTE: Unless the dump_modify sort option is invoked, the lines of atom information written to dump files (typically one line per atom) will be in an indeterminate order for each snapshot. This is even true when running on a single processor, if the atom_modify sort option is on, which it is by default. In this case atoms are re-ordered periodically during a simulation, due to spatial sorting. It is also true when running in parallel, because data for a single snapshot is collected from multiple processors.

For the atom, custom, cfg, and local styles, sorting is off by default. For the dcd, xtc, xyz, and molfile styles, sorting by atom ID is on by default. See the dump_modify doc page for details.

The style keyword determines what atom quantities are written to the file and in what format. Settings made via the dump_modify command can also alter the format of individual values and the file itself.

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The *atom*, *local*, and *custom* styles create files in a simple text format that is self-explanatory when viewing a dump file. Many of the LAMMPS post-processing tools, including Pizza.py, work with this format, as does the rerun command.

For post-processing purposes the *atom* and *custom* text files are self-describing in the following sense.

The dimensions of the simulation box are included in each snapshot. For an orthogonal simulation box this information is is formatted as:

```
ITEM: BOX BOUNDS xx yy zz
xlo xhi
ylo yhi
zlo zhi
```

where xlo, xhi are the maximum extents of the simulation box in the x-dimension, and similarly for y and z. The "xx yy zz" represent 6 characters that encode the style of boundary for each of the 6 simulation box boundaries (xlo, xhi and ylo, yhi and zlo, zhi). Each of the 6 characters is either p = periodic, f = fixed, s = shrink wrap, or m = shrink wrapped with a minimum value. See the boundary command for details.

For triclinic simulation boxes (non-orthogonal), an orthogonal bounding box which encloses the triclinic simulation box is output, along with the 3 tilt factors (xy, xz, yz) of the triclinic box, formatted as follows:

```
ITEM: BOX BOUNDS xy xz yz xx yy zz
xlo_bound xhi_bound xy
ylo_bound yhi_bound xz
zlo_bound zhi_bound yz
```

The presence of the text "xy xz yz" in the ITEM line indicates that the 3 tilt factors will be included on each of the 3 following lines. This bounding box is convenient for many visualization programs. The meaning of the 6 character flags for "xx yy zz" is the same as above.

Note that the first two numbers on each line are now xlo_bound instead of xlo, etc, since they represent a bounding box. See this section of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, simple formulas for how the 6 bounding box extents (xlo_bound, xhi_bound, etc) are calculated from the triclinic parameters, and how to transform those parameters to and from other commonly used triclinic representations.

The "ITEM: ATOMS" line in each snapshot lists column descriptors for the per-atom lines that follow. For example, the descriptors would be "id type xs ys zs" for the default atom style, and would be the atom attributes you specify in the dump command for the custom style.

For style atom, atom coordinates are written to the file, along with the atom ID and atom type. By default, atom coords are written in a scaled format (from 0 to 1). I.e. an x value of 0.25 means the atom is at a location 1/4 of the distance from xlo to xhi of the box boundaries. The format can be changed to unscaled coords via the dump_modify settings. Image flags can also be added for each atom via dump_modify.

Style custom allows you to specify a list of atom attributes to be written to the dump file for each atom. Possible attributes are listed above and will appear in the order specified. You cannot specify a quantity that is not defined for a particular simulation - such as q for atom style bond, since that atom style doesn't assign charges. Dumps occur at the very end of a timestep, so atom attributes will include effects due to fixes that are applied during the timestep. An explanation of the possible dump custom attributes is given below.

For style local, local output generated by computes and fixes is used to generate lines of output that is written to the dump file. This local data is typically calculated by each processor based on the atoms it owns, but there may be zero or more entities per atom, e.g. a list of bond distances. An explanation of the possible dump local
attributes is given below. Note that by using input from the `compute property/local` command with `dump local`, it is possible to generate information on bonds, angles, etc that can be cut and pasted directly into a data file read by the `read_data` command.

Style `cfg` has the same command syntax as style `custom` and writes extended CFG format files, as used by the AtomEye visualization package. Since the extended CFG format uses a single snapshot of the system per file, a wildcard "*" must be included in the filename, as discussed below. The list of atom attributes for style `cfg` must begin with either "id type xs ys zs" or "id type xsu ysu zsu" or since these quantities are needed to write the CFG files in the appropriate format (though the "id" and "type" fields do not appear explicitly in the file). Any remaining attributes will be stored as "auxiliary properties" in the CFG files. Note that you will typically want to use the `dump_modify element` command with CFG-formatted files, to associate element names with atom types, so that AtomEye can render atoms appropriately. When unwrapped coordinates `xsu`, `ysu`, and `zsu` are requested, the nominal AtomEye periodic cell dimensions are expanded by a large factor `UNWRAPEXPAND = 10.0`, which ensures atoms that are displayed correctly for up to `UNWRAPEXPAND/2` periodic boundary crossings in any direction. Beyond this, AtomEye will rewrap the unwrapped coordinates. The expansion causes the atoms to be drawn farther away from the viewer, but it is easy to zoom the atoms closer, and the interatomic distances are unaffected.

The `dcd` style writes DCD files, a standard atomic trajectory format used by the CHARMM, NAMD, and XPlor molecular dynamics packages. DCD files are binary and thus may not be portable to different machines. The number of atoms per snapshot cannot change with the `dcd` style. The `unwrap` option of the `dump_modify` command allows DCD coordinates to be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed through a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

The `xtc` style writes XTC files, a compressed trajectory format used by the GROMACS molecular dynamics package, and described here. The precision used in XTC files can be adjusted via the `dump_modify` command. The default value of 1000 means that coordinates are stored to 1/1000 nanometer accuracy. XTC files are portable binary files written in the NFS XDR data format, so that any machine which supports XDR should be able to read them. The number of atoms per snapshot cannot change with the `xtc` style. The `unwrap` option of the `dump_modify` command allows XTC coordinates to be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed thru a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

The `xyz` style writes XYZ files, which is a simple text-based coordinate format that many codes can read. Specifically it has a line with the number of atoms, then a comment line that is usually ignored followed by one line per atom with the atom type and the x-, y-, and z-coordinate of that atom. You can use the `dump_modify element` option to change the output from using the (numerical) atom type to an element name (or some other label). This will help many visualization programs to guess bonds and colors.

Note that `atom`, `custom`, `dcd`, `xtc`, and `xyz` style dump files can be read directly by VMD (a popular molecular viewing program). See `Section tools` of the manual and the `tools/lmp2vmd/README.txt` file for more information about support in VMD for reading and visualizing LAMMPS dump files.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the `dump_modify first` command, which can be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the `dump_modify every` command (not allowed for `dcd` style). The `dump_modify every` command also allows a variable to be used to
determine the sequence of timesteps on which dump files are written.

The specified filename determines how the dump file(s) is written. The default is to write one large text file, which is opened when the dump command is invoked and closed when an undump command is used or when LAMMPS exits. For the dcd and xtc styles, this is a single large binary file.

Dump filenames can contain two wildcard characters. If a "*" character appears in the filename, then one file per snapshot is written and the "*" character is replaced with the timestep value. For example, tmp.dump.* becomes tmp.dump.0, tmp.dump.10000, tmp.dump.20000, etc. This option is not available for the dcd and xtc styles. Note that the dump_modify pad command can be used to insure all timestep numbers are the same length (e.g. 00010), which can make it easier to read a series of dump files in order by some post-processing tools.

If a "%" character appears in the filename, then one file is written for each processor and the "%" character is replaced with the processor ID from 0 to P-1. For example, tmp.dump.% becomes tmp.dump.0, tmp.dump.1, ... tmp.dump.P-1, etc. This creates smaller files and can be a fast mode of output on parallel machines that support parallel I/O for output. This option is not available for the dcd, xtc, and xyz styles.

Note that the "*" and "%" characters can be used together to produce a large number of small dump files!

If the filename ends with ".bin", the dump file (or files, if "*" or "%" is also used) is written in binary format. A binary dump file will be about the same size as a text version, but will typically write out much faster. Of course, when post-processing, you will need to convert it back to text format (see the binary2txt tool) or write your own code to read the binary file. The format of the binary file can be understood by looking at the tools/binary2txt.cpp file. This option is only available for the atom and custom styles.

If the filename ends with ".gz", the dump file (or files, if "*" or "%" is also used) is written in gzipped format. A gzipped dump file will be about 3x smaller than the text version, but will also take longer to write. This option is not available for the dcd and xtc styles.

This section explains the local attributes that can be specified as part of the local style.

The index attribute can be used to generate an index number from 1 to N for each line written into the dump file, where N is the total number of local datums from all processors, or lines of output that will appear in the snapshot. Note that because data from different processors depend on what atoms they currently own, and atoms migrate between processor, there is no guarantee that the same index will be used for the same info (e.g. a particular bond) in successive snapshots.

The c_ID and c_ID[N] attributes allow local vectors or arrays calculated by a compute to be output. The ID in the attribute should be replaced by the actual ID of the compute that has been defined previously in the input script. See the compute command for details. There are computes for calculating local information such as indices, types, and energies for bonds and angles.

Note that computes which calculate global or per-atom quantities, as opposed to local quantities, cannot be output in a dump local command. Instead, global quantities can be output by the thermo_style custom command, and per-atom quantities can be output by the dump custom command.

If c_ID is used as a attribute, then the local vector calculated by the compute is printed. If c_ID[N] is used, then N must be in the range from 1-M, which will print the Nth column of the M-length local array calculated by the compute.

The f_ID and f_ID[N] attributes allow local vectors or arrays calculated by a fix to be output. The ID in the attribute should be replaced by the actual ID of the fix that has been defined previously in the input script.
If \( f_{ID} \) is used as a attribute, then the local vector calculated by the fix is printed. If \( f_{ID}[N] \) is used, then \( N \) must be in the range from 1-M, which will print the \( N \)th column of the M-length local array calculated by the fix.

Here is an example of how to dump bond info for a system, including the distance and energy of each bond:

```bash
compute 1 all property/local batom1 batom2 btype
compute 2 all bond/local dist eng
dump 1 all local 1000 tmp.dump index c_11 c_12 c_13 c_21 c_22
```

This section explains the atom attributes that can be specified as part of the \textit{custom} and \textit{cfg} styles.


\textit{Id} is the atom ID. \textit{Mol} is the molecule ID, included in the data file for molecular systems. \textit{Type} is the atom type. \textit{Element} is typically the chemical name of an element, which you must assign to each type via the \texttt{dump_modify element} command. More generally, it can be any string you wish to associated with an atom type. \textit{Mass} is the atom mass. \textit{Vx}, \textit{vy}, \textit{vz}, \textit{fx}, \textit{fy}, \textit{fz}, and \textit{q} are components of atom velocity and force and atomic charge.

There are several options for outputting atom coordinates. The \textit{x}, \textit{y}, \textit{z} attributes write atom coordinates "unscaled", in the appropriate distance \textit{units} (Angstroms, sigma, etc). Use \textit{xs}, \textit{ys}, \textit{zs} if you want the coordinates "scaled" to the box size, so that each value is 0.0 to 1.0. If the simulation box is triclinic (tilted), then all atom coords will still be between 0.0 and 1.0. Use \textit{xu}, \textit{yu}, \textit{zu} if you want the coordinates "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed thru a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that using \textit{xu}, \textit{yu}, \textit{zu} means that the coordinate values may be far outside the box bounds printed with the snapshot. Using \textit{xsu}, \textit{ysu}, \textit{zsu} is similar to using \textit{xu}, \textit{yu}, \textit{zu}, except that the unwrapped coordinates are scaled by the box size. Atoms that have passed through a periodic boundary will have the corresponding coordinate increased or decreased by 1.0.

The image flags can be printed directly using the \textit{ix}, \textit{iy}, \textit{iz} attributes. The \texttt{dump_modify} command describes in more detail what is meant by scaled vs unscaled coordinates and the image flags.

The \textit{mux}, \textit{muy}, \textit{muz} attributes are specific to dipolar systems defined with an atom style of \textit{dipole}. They give the orientation of the atom's point dipole moment. The \textit{mu} attribute gives the magnitude of the atom's dipole moment.

The \textit{radius} and \textit{diameter} attributes are specific to extended spherical particles that have a finite size, such as those defined with an atom style of \textit{sphere}.

The \textit{omegax}, \textit{omegay}, and \textit{omegaz} attributes are specific to extended spherical or aspherical particles that have an angular velocity. Only certain atom styles, such as \textit{sphere} define this quantity.

The \textit{angmomx}, \textit{angmomy}, and \textit{angmomz} attributes are specific to extended aspherical particles that have an angular momentum. Only the \textit{ellipsoid} atom style defines this quantity.

The \textit{tqx}, \textit{tqy}, \textit{tqz} attributes are for extended spherical or aspherical particles that can sustain a rotational torque due to interactions with other particles.

The \textit{spin}, \textit{eradius}, \textit{erel}, and \textit{erforce} attributes are for particles that represent nuclei and electrons modeled with the electronic force field (EFF). See \texttt{atom_style electron} and \texttt{pair_style eff} for more details.

The \textit{c_ID} and \textit{c_ID[N]} attributes allow per-atom vectors or arrays calculated by a \texttt{compute} to be output. The ID in the attribute should be replaced by the actual ID of the compute that has been defined previously in the input script. See the \texttt{compute} command for details. There are computes for calculating the per-atom energy, stress, centro-symmetry parameter, and coordination number of individual atoms.
Note that computes which calculate global or local quantities, as opposed to per-atom quantities, cannot be output in a dump custom command. Instead, global quantities can be output by the `thermo_style` command, and local quantities can be output by the `dump local` command.

If `c_ID` is used as a attribute, then the per-atom vector calculated by the compute is printed. If `c_ID[N]` is used, then N must be in the range from 1-M, which will print the Nth column of the M-length per-atom array calculated by the compute.

The `f_ID` and `f_ID[N]` attributes allow vector or array per-atom quantities calculated by a `fix` to be output. The ID in the attribute should be replaced by the actual ID of the fix that has been defined previously in the input script. The `fix ave/atom` command is one that calculates per-atom quantities. Since it can time-average per-atom quantities produced by any `compute`, `fix`, or atom-style `variable`, this allows those time-averaged results to be written to a dump file.

If `f_ID` is used as a attribute, then the per-atom vector calculated by the fix is printed. If `f_ID[N]` is used, then N must be in the range from 1-M, which will print the Nth column of the M-length per-atom array calculated by the fix.

The `v_name` attribute allows per-atom vectors calculated by a `variable` to be output. The name in the attribute should be replaced by the actual name of the variable that has been defined previously in the input script. Only an atom-style variable can be referenced, since it is the only style that generates per-atom values. Variables of style `atom` can reference individual atom attributes, per-atom atom attributes, thermodynamic keywords, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of creating quantities to output to a dump file.

See Section modify of the manual for information on how to add new compute and fix styles to LAMMPS to calculate per-atom quantities which could then be output into dump files.

**Restrictions:**

To write gzipped dump files, you must compile LAMMPS with the -DLAMMPS_GZIP option - see the Making LAMMPS section of the documentation.

The `xtc` style is part of the XTC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. This is because some machines may not support the low-level XDR data format that XTC files are written with, which will result in a compile-time error when a low-level include file is not found. Putting this style in a package makes it easy to exclude from a LAMMPS build for those machines. However, the XTC package also includes two compatibility header files and associated functions, which should be a suitable substitute on machines that do not have the appropriate native header files. This option can be invoked at build time by adding -DLAMMPS_XDR to the CCFLAGS variable in the appropriate low-level Makefile, e.g. src/MAKE/Makefile.foo. This compatibility mode has been tested successfully on Cray XT3/XT4/XT5 and IBM BlueGene/L machines and should also work on IBM BG/P, and Windows XP/Vista/7 machines.

**Related commands:**

`dump image`, `dump_modify`, `undump`

**Default:**

The defaults for the image style are listed on the `dump image` doc page.
dump image command

Syntax:

dump ID group-ID image N file color diameter keyword value ...

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be imaged
- image = style of dump command (other styles atom or cfg or dcd or xtc or xyz or local or custom are discussed on the dump doc page)
- N = dump every this many timesteps
- file = name of file to write image to
- color = atom attribute that determines color of each atom
- diameter = atom attribute that determines size of each atom
- zero or more keyword/value pairs may be appended
- keyword = adiam or atom or bond or size or view or center or up or zoom or persp or box or axes or shiny or ssao

adiam value = number = numeric value for atom diameter (distance units)
atom = yes/no = do or do not draw atoms
bond values = color width = color and width of bonds
  color = atom or type or none
  width = number or atom or type or none
  number = numeric value for bond width (distance units)
size values = width height = size of images
  width = width of image in # of pixels
  height = height of image in # of pixels
view values = theta phi = view of simulation box
  theta = view angle from +z axis (degrees)
  phi = azimuthal view angle (degrees)
  theta or phi can be a variable (see below)
center values = flag Cx Cy Cz = center point of image
  flag = "s" for static, "d" for dynamic
  Cx,Cy,Cz = center point of image as fraction of box dimension (0.5 = center of box)
  Cx,Cy,Cz can be variables (see below)
up values = Ux Uy Uz = direction that is "up" in image
  Ux,Uy,Uz = components of up vector
  Ux,Uy,Uz can be variables (see below)
zoom value = zfactor = size that simulation box appears in image
  zfactor = scale image size by factor > 1 to enlarge, factor <1 to shrink
  zfactor can be a variable (see below)
persp value = pfactor = amount of "perspective" in image
  pfactor = amount of perspective (0 = none, <1 = some, > 1 = highly skewed)
pfactor can be a variable (see below)
box values = yes/no diam = draw outline of simulation box
  yes/no = do or do not draw simulation box lines
  diam = diameter of box lines as fraction of shortest box length
axes values = yes/no length diam = draw xyz axes
  yes/no = do or do not draw xyz axes lines next to simulation box
  length = length of axes lines as fraction of respective box lengths
  diam = diameter of axes lines as fraction of shortest box length
shiny value = sfactor = shinyness of spheres and cylinders
  sfactor = shinyness of spheres and cylinders from 0.0 to 1.0
ssao value = yes/no seed dfactor = SSAO depth shading
  yes/no = turn depth shading on/off
  seed = random # seed (positive integer)
dfactor = strength of shading from 0.0 to 1.0
Examples:

dump myDump all image 100 dump.*.jpg type type

Description:

Dump a high-quality ray-traced image of the atom configuration every N timesteps as either a JPG or PPM file. A series of such images can easily be converted into an animated movie of your simulation; see further details below. Other dump styles store snapshots of numerical data associated with atoms in various formats, as discussed on the dump doc page.

Here are two sample images, rendered as 1024x1024 JPG files. Click to see the full-size images:

![Sample Images](image1.jpg) ![Sample Images](image2.jpg)

Only atoms in the specified group are rendered in the image. The dump_modify region and thresh commands can also alter what atoms are included in the image.

The filename suffix determines whether a JPG or PPM file is created. If the suffix is ".jpg" or ".jpeg", then a JPG file is created, else a PPM file is created, which is a text-based format. To write out JPG files, you must build LAMMPS with a JPEG library. See this section of the manual for instructions on how to do this.

IMPORTANT NOTE: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom in the image may be slightly outside the simulation box.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the dump_modify first command, which can be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the dump_modify every command.

Dump image filenames must contain a wildcard character "*", so that one image file per snapshot is written. The "*" character is replaced with the timestep value. For example, tmp.dump.*.jpg becomes tmp.dump.0.jpg, tmp.dump.10000.jpg, tmp.dump.20000.jpg, etc. Note that the dump_modify pad command can be used to insure all timestep numbers are the same length (e.g. 00010), which can make it easier to convert a series of images into a movie in the correct ordering.

The color and diameter settings determine the color and size of atoms rendered in the image. They can be any atom attribute defined for the dump custom command, including type and element. This includes per-atom
quantities calculated by a compute, fix, or variable, which are prefixed by "c_", "f_", or "v_" respectively. Note that the diameter setting can be overridden with a numeric value by the optional adiam keyword, in which case you can specify the diameter setting with any valid atom attribute.

If type is specified for the color setting, then the color of each atom is determined by its atom type. By default the mapping of types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for types > 6. This mapping can be changed by the dump_modify acolor command.

If type is specified for the diameter setting then the diameter of each atom is determined by its atom type. By default all types have diameter 1.0. This mapping can be changed by the dump_modify adiam command.

If element is specified for the color and/or diameter setting, then the color and/or diameter of each atom is determined by which element it is, which in turn is specified by the element-to-type mapping specified by the "dump_modify element" command. By default every atom type is C (carbon). Every element has a color and diameter associated with it, which is the same as the colors and sizes used by the AtomEye visualization package.

If other atom attributes are used for the color or diameter settings, they are interpreted in the following way.

If "vx", for example, is used as the color setting, then the color of the atom will depend on the x-component of its velocity. The association of a per-atom value with a specific color is determined by a "color map", which can be specified via the dump_modify command. The basic idea is that the atom-attribute will be within a range of values, and every value within the range is mapped to a specific color. Depending on how the color map is defined, that mapping can take place via interpolation so that a value of -3.2 is halfway between "red" and "blue", or discretely so that the value of -3.2 is "orange".

If "vx", for example, is used as the diameter setting, then the atom will be rendered using the x-component of its velocity as the diameter. If the per-atom value <= 0.0, then the atom will not be drawn. Note that finite-size spherical particles, as defined by atom_style sphere define a per-particle radius or diameter, which can be used as the diameter setting.

The various keywords listed above control how the image is rendered. As listed below, all of the keywords have defaults, most of which you will likely not need to change. The dump modify also has options specific to the dump image style, particularly for assigning colors to atoms, bonds, and other image features.

The adiam keyword allows you to override the diameter setting to a per-atom attribute with a specified numeric value. All atoms will be drawn with that diameter, e.g. 1.5, which is in whatever distance units the input script defines, e.g. Angstroms.

The atom keyword allow you to turn off the drawing of all atoms, if the specified value is no.

The bond keyword allows you to alter how bonds are drawn. A bond is only drawn if both atoms in the bond are being drawn due to being in the specified group and due to other selection criteria (e.g. region, threshold settings of the dump_modify command). By default, bonds are drawn if they are defined in the input data file as read by the read_data command. Using none for both the bond color and width value will turn off the drawing of
all bonds.

If *atom* is specified for the bond *color* value, then each bond is drawn in 2 halves, with the color of each half being the color of the atom at that end of the bond.

If *type* is specified for the *color* value, then the color of each bond is determined by its bond type. By default the mapping of bond types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for bond types > 6. This mapping can be changed by the *dump_modify bcolor* command.

The bond *width* value can be a numeric value or *atom* or *type* (or *none* as indicated above).

If a numeric value is specified, then all bonds will be drawn as cylinders with that diameter, e.g. 1.0, which is in whatever distance *units* the input script defines, e.g. Angstroms.

If *atom* is specified for the *width* value, then each bond will be drawn with a width corresponding to the minimum diameter of the 2 atoms in the bond.

If *type* is specified for the *width* value then the diameter of each bond is determined by its bond type. By default all types have diameter 0.5. This mapping can be changed by the *dump_modify bdiam* command.

The *size* keyword sets the width and height of the created images, i.e. the number of pixels in each direction.

The *view*, *center*, *up*, *zoom*, and *persp* values determine how 3d simulation space is mapped to the 2d plane of the image. Basically they control how the simulation box appears in the image.

All of the *view*, *center*, *up*, *zoom*, and *persp* values can be specified as numeric quantities, whose meaning is explained below. Any of them can also be specified as an *equal-style variable*, by using v_name as the value, where "name" is the variable name. In this case the variable will be evaluated on the timestep each image is created to create a new value. If the equal-style variable is time-dependent, this is a means of changing the way the simulation box appears from image to image, effectively doing a pan or fly-by view of your simulation.

The *view* keyword determines the viewpoint from which the simulation box is viewed, looking towards the *center* point. The *theta* value is the vertical angle from the +z axis, and must be an angle from 0 to 180 degrees. The *phi* value is an azimuthal angle around the z axis and can be positive or negative. A value of 0.0 is a view along the +x axis, towards the *center* point. If *theta* or *phi* are specified via variables, then the variable values should be in degrees.

The *center* keyword determines the point in simulation space that will be at the center of the image. Cx, Cy, and Cz are specified as fractions of the box dimensions, so that (0.5,0.5,0.5) is the center of the simulation box. These values do not have to be between 0.0 and 1.0, if you want the simulation box to be offset from the center of the image. Note, however, that if you choose strange values for Cx, Cy, or Cz you may get a blank image. Internally, Cx, Cy, and Cz are converted into a point in simulation space. If *flag* is set to "s" for static, then this conversion is done once, at the time the dump command is issued. If *flag* is set to "d" for dynamic then the conversion is performed every time a new image is created. If the box size or shape is changing, this will adjust the center point.
in simulation space.

The *up* keyword determines what direction in simulation space will be "up" in the image. Internally it is stored as a vector that is in the plane perpendicular to the view vector implied by the *theta* and *phi* values, and which is also in the plane defined by the view vector and user-specified up vector. Thus this internal vector is computed from the user-specified *up* vector as

\[
up_{\text{internal}} = \text{view} \times (up \times \text{view})
\]

This means the only restriction on the specified *up* vector is that it cannot be parallel to the *view* vector, implied by the *theta* and *phi* values.

The *zoom* keyword scales the size of the simulation box as it appears in the image. The default *zfactor* value of 1 should display an image mostly filled by the atoms in the simulation box. A *zfactor* > 1 will make the simulation box larger; a *zfactor* < 1 will make it smaller. *Zfactor* must be a value > 0.0.

The *persp* keyword determines how much depth perspective is present in the image. Depth perspective makes lines that are parallel in simulation space appear non-parallel in the image. A *pfactor* value of 0.0 means that parallel lines will meet at infinity (1.0/pfactor), which is an orthographic rendering with no perspective. A *pfactor* value between 0.0 and 1.0 will introduce more perspective. A *pfactor* value > 1 will create a highly skewed image with a large amount of perspective.

**IMPORTANT NOTE:** The *persp* keyword is not yet supported as an option.

The *box* keyword determines how the simulation box boundaries are rendered as thin cylinders in the image. If *no* is set, then the box boundaries are not drawn and the *diam* setting is ignored. If *yes* is set, the 12 edges of the box are drawn, with a diameter that is a fraction of the shortest box length in x,y,z (for 3d) or x,y (for 2d). The color of the box boundaries can be set with the `dump_modify boxcolor` command.

The *axes* keyword determines how the coordinate axes are rendered as thin cylinders in the image. If *no* is set, then the axes are not drawn and the *length* and *diam* settings are ignored. If *yes* is set, 3 thin cylinders are drawn to represent the x,y,z axes in colors red,green,blue. The origin of these cylinders will be offset from the lower left corner of the box by 10%. The *length* setting determines how long the cylinders will be as a fraction of the respective box lengths. The *diam* setting determines their thickness as a fraction of the shortest box length in x,y,z (for 3d) or x,y (for 2d).

The *shiny* keyword determines how shiny the objects rendered in the image will appear. The *sfactor* value must be a value 0.0 <= *sfactor* <= 1.0, where *sfactor* = 1 is a highly reflective surface and *sfactor* = 0 is a rough non-shiny surface.

The *ssao* keyword turns on/off a screen space ambient occlusion (SSAO) model for depth shading. If *yes* is set, then atoms further away from the viewer are darkened via a randomized process, which is perceived as depth. The calculation of this effect can increase the cost of computing the image by roughly 2x. The strength of the effect can be scaled by the *dfactor* parameter. If *no* is set, no depth shading is performed.

A series of JPG or PPM images can be converted into a movie file and then played as a movie using commonly available tools.

Convert JPG or PPM files into an animated GIF or MPEG or other movie file:

- a) Use the ImageMagick convert program.
% convert *.jpg foo.gif
% convert -loop 1 *.ppm foo.mpg

• b) Use QuickTime.

Select "Open Image Sequence" under the File menu Load the images into QuickTime to animate them
Select "Export" under the File menu Save the movie as a QuickTime movie (*.mov) or in another format
• c) Windows-based tool.

If someone tells us how to do this via a common Windows-based tool, we'll post the instructions here.

Play the movie:

• a) Use your browser to view an animated GIF movie.

Select "Open File" under the File menu Load the animated GIF file
• b) Use the freely available mplayer tool to view an MPEG movie.

% mplayer foo.mpg
• c) Use the Pizza.py animate tool, which works directly on a series of image files.

    a = animate("foo*.jpg")

• d) QuickTime and other Windows-based media players can obviously play movie files directly.

See Section modify of the manual for information on how to add new compute and fix styles to LAMMPS to
calculate per-atom quantities which could then be output into dump files.

Restrictions:

To write JPG images, you must use a -DLAMMPS_JPEG switch when building LAMMPS and link with a JPEG
library. See the Making LAMMPS section of the documentation for details.

Related commands:

dump, dump_modify, undump

Default:

The defaults for the keywords are as follows:

• adiam = not specified (use diameter setting)
• atom = yes
• bond = none none (if no bonds in system)
• bond = atom 0.5 (if bonds in system)
• size = 512 512
• view = 60 30 (for 3d)
• view = 0 0 (for 2d)
• center = s 0.5 0.5 0.5
• up = 0 0 1 (for 3d)
• up = 0 1 0 (for 2d)
• zoom = 1.0
• persp = 0.0
• box = yes 0.02
• axes = no 0.0 0.0
• shiny = 1.0
• ssao = no
dump_modify command

Syntax:

dump_modify dump-ID keyword values ...

- dump-ID = ID of dump to modify
- one or more keyword/value pairs may be appended
- keyword = acolor or adiam or amap or append or bcolor or bdiam or backcolor or boxcolor or color or every or flush or format or image or label or precision or region or scale or sort or thresh or unwrap

- acolor args = type color
  type = atom type or range of types (see below)
  color = name of color or color1/color2/...

- adiam args = type diam
  type = atom type or range of types (see below)
  diam = diameter of atoms of that type (distance units)

- amap args = lo hi style delta N entry1 entry2 ... entryN
  lo = number or min = lower bound of range of color map
  hi = number or max = upper bound of range of color map
  style = 2 letters = "c" or "d" or "s" plus "a" or "f"
  "c" for continuous
  "d" for discrete
  "s" for sequential
  "a" for absolute
  "f" for fractional
  delta = binsize (only used for style "s", otherwise ignored)
  binsize = range is divided into bins of this width
  N = # of subsequent entries
  entry = value color (for continuous style)
  value = number or min or max = single value within range
  color = name of color used for that value

- append arg = yes or no

- bcolor args = type color
  type = bond type or range of types (see below)
  color = name of color or color1/color2/...

- bdiam args = type diam
  type = bond type or range of types (see below)
  diam = diameter of bonds of that type (distance units)

- backcolor arg = color
  color = name of color for background

- boxcolor arg = color
  color = name of color for box lines

- color args = name R G B
  name = name of color
  R,G,B = red/green/blue numeric values from 0.0 to 1.0

- element args = E1 E2 ... EN, where N = # of atom types
  E1,...,EN = element name, e.g. C or Fe or Ga

- every arg = N
  N = dump every this many timesteps

- first arg = yes or no

- format arg = C-style format string for one line of output

- flush arg = yes or no
image arg = yes or no
label arg = string
    string = character string (e.g. BONDS) to use in header of dump local file
pad arg = Nchar = # of characters to convert timestep to
precision arg = power-of-10 value from 10 to 1000000
region arg = region-ID or "none"
scale arg = yes or no
sort arg = off or id or N or -N
    off = no sorting of per-atom lines within a snapshot
    id = sort per-atom lines by atom ID
    N = sort per-atom lines in ascending order by the Nth column
    -N = sort per-atom lines in descending order by the Nth column
thresh args = attribute operation value
    attribute = same attributes (x,fy,etotal,sxx,etc) used by dump custom style
    operation = "" or ">=" or "==" or ">="
    value = numeric value to compare to
    these 3 args can be replaced by the word "none" to turn off thresholding
unwrap arg = yes or no

Examples:

dump_modify 1 format "%d %d %20.15g %g %g" scale yes
dump_modify myDump image yes scale no flush yes
dump_modify 1 region mySphere thresh x <0.0 thresh epair >= 3.2
dump_modify xtcdump precision 10000
dump_modify 1 every 1000
dump_modify 1 every v_myVar
dump_modify 1 amap min max cf 0.0 3 min green 0.5 yellow max blue boxcolor red

Description:

Modify the parameters of a previously defined dump command. Not all parameters are relevant to all dump styles.

The acolor keyword applies only to the dump image style. It can be used with the dump image command, when its atom color setting is type, to set the color that atoms of each type will be drawn in the image.

The specified type should be an integer from 1 to Ntypes = the number of atom types. A wildcard asterisk can be used in place of or in conjunction with the type argument to specify a range of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

The specified color can be a single color which is any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option. Or it can be two or more colors separated by a "/" character, e.g. red/green/blue. In the former case, that color is assigned to all the specified atom types. In the latter case, the list of colors are assigned in a round-robin fashion to each of the specified atom types.

The adiam keyword applies only to the dump image style. It can be used with the dump image command, when its atom diameter setting is type, to set the size that atoms of each type will be drawn in the image. The specified type should be an integer from 1 to Ntypes. As with the acolor keyword, a wildcard asterisk can be used as part of the type argument to specify a range of atom types. The specified diam is the size in whatever distance units the input script is using, e.g. Angstroms.

The amap keyword applies only to the dump image style. It can be used with the dump image command, with its atom keyword, when its atom setting is an atom-attribute, to setup a color map. The color map is used to assign a specific RGB (red/green/blue) color value to an individual atom when it is drawn, based on the atom's attribute,
which is a numeric value, e.g. its x-component of velocity if the atom-attribute "vx" was specified.

The basic idea of a color map is that the atom-attribute will be within a range of values, and that range is associated with a a series of colors (e.g. red, blue, green). An atom's specific value (vx = -3.2) can then mapped to the series of colors (e.g. halfway between red and blue), and a specific color is determined via an interpolation procedure.

There are many possible options for the color map, enabled by the amap keyword. Here are the details.

The lo and hi settings determine the range of values allowed for the atom attribute. If numeric values are used for lo and/or hi, then values that are lower/higher than that value are set to the value. I.e. the range is static. If lo is specified as min or hi as max then the range is dynamic, and the lower and/or upper bound will be calculated each time an image is drawn, based on the set of atoms being visualized.

The style setting is two letters, such as "ca". The first letter is either "c" for continuous, "d" for discrete, or "s" for sequential. The second letter is either "a" for absolute, or "f" for fractional.

A continuous color map is one in which the color changes continuously from value to value within the range. A discrete color map is one in which discrete colors are assigned to sub-ranges of values within the range. A sequential color map is one in which discrete colors are assigned to a sequence of sub-ranges of values covering the entire range.

An absolute color map is one in which the values to which colors are assigned are specified explicitly as values within the range. A fractional color map is one in which the values to which colors are assigned are specified as a fractional portion of the range. For example if the range is from -10.0 to 10.0, and the color red is to be assigned to atoms with a value of 5.0, then for an absolute color map the number 5.0 would be used. But for a fractional map, the number 0.75 would be used since 5.0 is 3/4 of the way from -10.0 to 10.0.

The delta setting must be specified for all styles, but is only used for the sequential style; otherwise the value is ignored. It specifies the bin size to use within the range for assigning consecutive colors to. For example, if the range is from -10.0 to 10.0 and a delta of 1.0 is used, then 20 colors will be assigned to the range. The first will be from -10.0 <= color1 < -9.0, then 2nd from -9.0 <= color2 < -8.0, etc.

The N setting is how many entries follow. The format of the entries depends on whether the color map style is continuous, discrete or sequential. In all cases the color setting can be any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option.

For continuous color maps, each entry has a value and a color. The value is either a number within the range of values or min or max. The value of the first entry must be min and the value of the last entry must be max. Any entries in between must have increasing values. Note that numeric values can be specified either as absolute numbers or as fractions (0.0 to 1.0) of the range, depending on the "a" or "f" in the style setting for the color map.

Here is how the entries are used to determine the color of an individual atom, given the value X of its atom attribute. X will fall between 2 of the entry values. The color of the atom is linearly interpolated (in each of the RGB values) between the 2 colors associated with those entries. For example, if X = -5.0 and the 2 surrounding entries are "red" at -10.0 and "blue" at 0.0, then the atom's color will be halfway between "red" and "blue", which happens to be "purple".

For discrete color maps, each entry has a lo and hi value and a color. The lo and hi settings are either numbers within the range of values or lo can be min or hi can be max. The lo and hi settings of the last entry must be min and max. Other entries can have any lo and hi values and the sub-ranges of different values can overlap. Note that numeric lo and hi values can be specified either as absolute numbers or as fractions (0.0 to 1.0) of the range,
depending on the "a" or "f" in the style setting for the color map.

Here is how the entries are used to determine the color of an individual atom, given the value X of its atom attribute. The entries are scanned from first to last. The first time that \(lo \leq X \leq hi\), \(X\) is assigned the color associated with that entry. You can think of the last entry as assigning a default color (since it will always be matched by \(X\)), and the earlier entries as colors that override the default. Also note that no interpolation of a color RGB is done. All atoms will be drawn with one of the colors in the list of entries.

For sequential color maps, each entry has only a color. Here is how the entries are used to determine the color of an individual atom, given the value \(X\) of its atom attribute. The range is partitioned into \(N\) bins of width \(binsize\). Thus \(X\) will fall in a specific bin from 1 to \(N\), say the \(M\)th bin. If it falls on a boundary between 2 bins, it is considered to be in the higher of the 2 bins. Each bin is assigned a color from the \(E\) entries. If \(E < N\), then the colors are repeated. For example if \(2\) entries with colors red and green are specified, then the odd numbered bins will be red and the even bins green. The color of the atom is the color of its bin. Note that the sequential color map is really a shorthand way of defining a discrete color map without having to specify where all the bin boundaries are.

The `append` keyword applies to all dump styles except `cfg` and `xtc` and `dcd`. It also applies only to text output files, not to binary or gzipped files. If specified as `yes`, then dump snapshots are appended to the end of an existing dump file. If specified as `no`, then a new dump file will be created which will overwrite an existing file with the same name. This keyword can only take effect if the `dump_modify` command is used after the `dump` command, but before the first command that causes dump snapshots to be output, e.g. a `run` or `minimize` command. Once the dump file has been opened, this keyword has no further effect.

The `bcolor` keyword applies only to the dump `image` style. It can be used with the `dump image` command, with its `bond` keyword, when its color setting is `type`, to set the color that bonds of each type will be drawn in the image.

The specified `type` should be an integer from 1 to \(N_{bondtypes} = \) the number of bond types. A wildcard asterisk can be used in place of or in conjunction with the `type` argument to specify a range of bond types. This takes the form "*" or "*n" or "n*" or "m*n". If \(N\) = the number of bond types, then an asterisk with no numeric values means all types from 1 to \(N\). A leading asterisk means all types from 1 to \(n\) (inclusive). A trailing asterisk means all types from \(n\) to \(N\) (inclusive). A middle asterisk means all types from \(m\) to \(n\) (inclusive).

The specified `color` can be a single color which is any of the 140 pre-defined colors (see below) or a color name defined by the `dump_modify` color option. Or it can be two or more colors separated by a '/' character, e.g. red/green/blue. In the former case, that color is assigned to all the specified bond types. In the latter case, the list of colors are assigned in a round-robin fashion to each of the specified bond types.

The `bdiam` keyword applies only to the dump `image` style. It can be used with the `dump image` command, with its `bond` keyword, when its diam setting is `type`, to set the diameter that bonds of each type will be drawn in the image. The specified `type` should be an integer from 1 to \(N_{bondtypes}\). As with the `bcolor` keyword, a wildcard asterisk can be used as part of the `type` argument to specify a range of bond types. The specified `diam` is the size in whatever distance `units` you are using, e.g. Angstroms.

The `backcolor` keyword applies only to the dump `image` style. It sets the background color of the images. The color name can be any of the 140 pre-defined colors (see below) or a color name defined by the `dump_modify` color option.

The `boxcolor` keyword applies only to the dump `image` style. It sets the color of the simulation box drawn around the atoms in each image. See the "dump image box" command for how to specify that a box be drawn. The color name can be any of the 140 pre-defined colors (see below) or a color name defined by the `dump_modify` color option.
The `color` keyword applies only to the `dump image` style. It allows definition of a new color name, in addition to the 140-predefined colors (see below), and associates 3 red/green/blue RGB values with that color name. The color name can then be used with any other `dump_modify` keyword that takes a color name as a value. The RGB values should each be floating point values between 0.0 and 1.0 inclusive.

When a color name is converted to RGB values, the user-defined color names are searched first, then the 140 pre-defined color names. This means you can also use the `color` keyword to overwrite one of the pre-defined color names with new RGB values.

The `element` keyword applies only to the the `dump cfg`, `xyz`, and `image` styles. It associates element names (e.g. H, C, Fe) with LAMMPS atom types. See the list of element names at the bottom of this page.

In the case of `dump cfg`, this allows the AtomEye visualization package to read the dump file and render atoms with the appropriate size and color.

In the case of `dump image`, the output images will follow the same AtomEye convention. An element name is specified for each atom type (1 to Ntype) in the simulation. The same element name can be given to multiple atom types.

In the case of `xyz` format dumps, there are no restrictions to what label can be used as an element name. Any whitespace separated text will be accepted.

The `every` keyword changes the dump frequency originally specified by the `dump` command to a new value. The every keyword can be specified in one of two ways. It can be a numeric value in which case it must be > 0. Or it can be an `equal-style variable`, which should be specified as `v_name`, where name is the variable name.

In this case, the variable is evaluated at the beginning of a run to determine the next timestep at which a dump snapshot will be written out. On that timestep, the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for `equal-style variables`, as examples of useful functions to use in this context. Other similar math functions could easily be added as options for `equal-style variables`. When using the variable option with the `every` keyword, you also need to use the `first` option if you want an initial snapshot written to the dump file. The `every` keyword cannot be used with the dump `dcd` style.

For example, the following commands will write snapshots at timesteps 0, 10, 20, 30, 100, 200, 300, 1000, 2000, etc:

```plaintext
variable        s equal logfreq(10,3,10)
dump            1 all atom 100 tmp.dump
dump_modify     1 every v_s first yes
```

The `first` keyword determines whether a dump snapshot is written on the very first timestep after the `dump` command is invoked. This will always occur if the current timestep is a multiple of N, the frequency specified in the `dump` command, including timestep 0. But if this is not the case, a dump snapshot will only be written if the setting of this keyword is `yes`. If it is `no`, which is the default, then it will not be written.

The `flush` keyword determines whether a flush operation is invoked after a dump snapshot is written to the dump file. A flush insures the output in that file is current (no buffering by the OS), even if LAMMPS halts before the simulation completes. Flashes cannot be performed with dump style `xtc`.

The text-based dump styles have a default C-style format string which simply specifies `%d` for integers and `%g` for real values. The `format` keyword can be used to override the default with a new C-style format string. Do not
include a trailing "\n" newline character in the format string. This option has no effect on the dcd and xtc dump styles since they write binary files. Note that for the cfg style, the first two fields (atom id and type) are not actually written into the CFG file, though you must include formats for them in the format string.

The image keyword applies only to the dump atom style. If the image value is yes, 3 flags are appended to each atom’s coords which are the absolute box image of the atom in each dimension. For example, an x image flag of -2 with a normalized coord of 0.5 means the atom is in the center of the box, but has passed thru the box boundary 2 times and is really 2 box lengths to the left of its current coordinate. Note that for dump style custom these various values can be printed in the dump file by using the appropriate atom attributes in the dump command itself.

The label keyword applies only to the dump local style. When it writes local informatoin, such as bond or angle topology to a dump file, it will use the specified label to format the header. By default this includes 2 lines:

```
ITEM: NUMBER OF ENTRIES
ITEM: ENTRIES ...
```

The word "ENTRIES" will be replaced with the string specified, e.g. BONDS or ANGLES.

The pad keyword only applies when the dump filename is specified with a wildcard "*" character which becomes the timestep. If pad is 0, which is the default, the timestep is converted into a string of unpadded length, e.g. 100 or 12000 or 2000000. When pad is specified with Nchar > 0, the string is padded with leading zeroes so they are all the same length = Nchar. For example, pad 7 would yield 0000100, 0012000, 2000000. This can be useful so that post-processing programs can easily read the files in ascending timestep order.

The precision keyword only applies to the dump xtc style. A specified value of N means that coordinates are stored to 1/N nanometer accuracy, e.g. for N = 1000, the coordinates are written to 1/1000 nanometer accuracy.

The region keyword only applies to the dump custom and cfg and image styles. If specified, only atoms in the region will be written to the dump file or included in the image. Only one region can be applied as a filter (the last one specified). See the region command for more details. Note that a region can be defined as the "inside" or "outside" of a geometric shape, and it can be the "union" or "intersection" of a series of simpler regions.

The scale keyword applies only to the dump atom style. A scale value of yes means atom coords are written in normalized units from 0.0 to 1.0 in each box dimension. If the simluation box is triclinic (tilted), then all atom coords will still be between 0.0 and 1.0. A value of no means they are written in absolute distance units (e.g. Angstroms or sigma).

The sort keyword determines whether lines of per-atom output in a snapshot are sorted or not. A sort value of off means they will typically be written in indeterminate order, either in serial or parallel. This is the case even in serial if the atom_modify sort option is turned on, which it is by default, to improve performance. A sort value of id means sort the output by atom ID. A sort value of N or -N means sort the output by the value in the Nth column of per-atom info in either ascending or descending order. The dump local style cannot be sorted by atom ID, since there are typically multiple lines of output per atom. Some dump styles, such as dcd and xtc, require sorting by atom ID to format the output file correctly.

IMPORTANT NOTE: Unless it is required by the dump style, sorting dump file output requires extra overhead in terms of CPU and communication cost, as well as memory, versus unsorted output.

The thresh keyword only applies to the dump custom and cfg and image styles. Multiple thresholds can be specified. Specifying "none" turns off all threshold criteria. If thresholds are specified, only atoms whose attributes meet all the threshold criteria are written to the dump file or included in the image. The possible

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attributes that can be tested for are the same as those that can be specified in the dump custom command, with the exception of the `element` attribute, since it is not a numeric value. Note that different attributes can be output by the dump custom command than are used as threshold criteria by the dump_modify command. E.g. you can output the coordinates and stress of atoms whose energy is above some threshold.

The `unwrap` keyword only applies to the dump `dcd` and `xtc` styles. If set to `yes`, coordinates will be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed thru a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

**Restrictions:** none

**Related commands:**

`dump`, `dump image`, `undump`

**Default:**

The option defaults are

- `acolor = * red/green/blue/yellow/aqua/cyan`
- `adiam = * 1.0`
- `amap = min max cf 2 min blue max red`
- `append = no`
- `bcolor = * red/green/blue/yellow/aqua/cyan`
- `bdiam = * 0.5`
- `backcolor = black`
- `boxcolor = yellow`
- `color = 140 color names are pre-defined as listed below`
- `element = "C"` for every atom type
- `every = whatever it was set to via the dump command`
- `first = no`
- `flush = yes`
- `format = %d and %g for each integer or floating point value`
- `image = no`
- `label = ENTRIES`
- `pad = 0`
- `precision = 1000`
- `region = none`
- `scale = yes`
- `sort = off for dump styles atom, custom, cfg, and local`
- `sort = id for dump styles dcd, xtc, and xyz`
- `thresh = none`
- `unwrap = no`

These are the standard 109 element names that LAMMPS pre-defines for use with the `dump image` and `dump_modify` commands.

- 1-10 = "H", "He", "Li", "Be", "B", "C", "N", "O", "F", "Ne"
These are the 140 colors that LAMMPS pre-defines for use with the dump image and dump_modify commands. Additional colors can be defined with the dump_modify color command. The 3 numbers listed for each name are the RGB (red/green/blue) values. Divide each value by 255 to get the equivalent 0.0 to 1.0 value.

<table>
<thead>
<tr>
<th>Name</th>
<th>RGB Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>aliceblue</td>
<td>240, 248, 255</td>
</tr>
<tr>
<td>antiquewhite</td>
<td>250, 235, 215</td>
</tr>
<tr>
<td>aqua</td>
<td>0, 255, 255</td>
</tr>
<tr>
<td>aquamarine</td>
<td>127, 255, 212</td>
</tr>
<tr>
<td>azure</td>
<td>240, 255, 255</td>
</tr>
<tr>
<td>beige</td>
<td>245, 245, 220</td>
</tr>
<tr>
<td>bisque</td>
<td>255, 228, 196</td>
</tr>
<tr>
<td>black</td>
<td>0, 0, 0</td>
</tr>
<tr>
<td>blanchedalmond</td>
<td>255, 255, 205</td>
</tr>
<tr>
<td>blue</td>
<td>0, 0, 255</td>
</tr>
<tr>
<td>blueviolet</td>
<td>138, 43, 226</td>
</tr>
<tr>
<td>brown</td>
<td>165, 42, 42</td>
</tr>
<tr>
<td>burlywood</td>
<td>222, 184, 135</td>
</tr>
<tr>
<td>cadetblue</td>
<td>95, 158, 160</td>
</tr>
<tr>
<td>chartreuse</td>
<td>127, 255, 0</td>
</tr>
<tr>
<td>chocolate</td>
<td>210, 105, 30</td>
</tr>
<tr>
<td>coral</td>
<td>255, 127, 80</td>
</tr>
<tr>
<td>cornflowerblue</td>
<td>100, 149, 237</td>
</tr>
<tr>
<td>cornsilk</td>
<td>255, 248, 220</td>
</tr>
<tr>
<td>crimson</td>
<td>220, 20, 60</td>
</tr>
<tr>
<td>cyan</td>
<td>0, 255, 255</td>
</tr>
<tr>
<td>darkblue</td>
<td>0, 0, 139</td>
</tr>
<tr>
<td>darkcyan</td>
<td>0, 139, 139</td>
</tr>
<tr>
<td>darkgoldenrod</td>
<td>184, 134, 11</td>
</tr>
<tr>
<td>darkgray</td>
<td>169, 169, 169</td>
</tr>
<tr>
<td>darkgreen</td>
<td>0, 100, 0</td>
</tr>
<tr>
<td>darkkhaki</td>
<td>189, 183, 107</td>
</tr>
<tr>
<td>darkmagenta</td>
<td>139, 0, 139</td>
</tr>
<tr>
<td>darkolivegreen</td>
<td>85, 107, 47</td>
</tr>
<tr>
<td>darkorange</td>
<td>255, 140, 0</td>
</tr>
<tr>
<td>darkorchid</td>
<td>153, 50, 204</td>
</tr>
<tr>
<td>darkred</td>
<td>139, 0, 0</td>
</tr>
<tr>
<td>darksalmon</td>
<td>233, 150, 122</td>
</tr>
<tr>
<td>darkseagreen</td>
<td>143, 188, 143</td>
</tr>
<tr>
<td>darkslateblue</td>
<td>72, 61, 139</td>
</tr>
<tr>
<td>darkslategray</td>
<td>47, 79, 79</td>
</tr>
<tr>
<td>darkturquoise</td>
<td>0, 206, 209</td>
</tr>
<tr>
<td>darkviolet</td>
<td>148, 0, 211</td>
</tr>
<tr>
<td>deepink</td>
<td>255, 20, 147</td>
</tr>
<tr>
<td>deepskyblue</td>
<td>0, 191, 255</td>
</tr>
<tr>
<td>dimgray</td>
<td>105, 105, 105</td>
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<tr>
<td>dodgerblue</td>
<td>30, 144, 255</td>
</tr>
<tr>
<td>firebrick</td>
<td>178, 34, 34</td>
</tr>
<tr>
<td>floralwhite</td>
<td>255, 20, 147</td>
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<tr>
<td>forestgreen</td>
<td>34, 139, 139</td>
</tr>
<tr>
<td>fuchsia</td>
<td>255, 0, 255</td>
</tr>
<tr>
<td>gainsboro</td>
<td>220, 220, 220</td>
</tr>
<tr>
<td>ghostwhite</td>
<td>248, 248, 255</td>
</tr>
<tr>
<td>gold</td>
<td>255, 215, 0</td>
</tr>
<tr>
<td>goldenrod</td>
<td>255, 215, 0</td>
</tr>
<tr>
<td>gray</td>
<td>128, 128, 128</td>
</tr>
<tr>
<td>green</td>
<td>0, 128, 0</td>
</tr>
<tr>
<td>greenyellow</td>
<td>173, 255, 47</td>
</tr>
<tr>
<td>honeydew</td>
<td>240, 255, 240</td>
</tr>
<tr>
<td>hotpink</td>
<td>255, 105, 180</td>
</tr>
<tr>
<td>indianred</td>
<td>205, 92, 92</td>
</tr>
<tr>
<td>indigo</td>
<td>75, 0, 130</td>
</tr>
<tr>
<td>ivory</td>
<td>255, 240, 240</td>
</tr>
<tr>
<td>khaki</td>
<td>240, 230, 140</td>
</tr>
<tr>
<td>lavenderblush</td>
<td>255, 240, 245</td>
</tr>
<tr>
<td>lawngreen</td>
<td>124, 252, 0</td>
</tr>
<tr>
<td>lemonchiffon</td>
<td>255, 250, 205</td>
</tr>
<tr>
<td>lightblue</td>
<td>173, 216, 230</td>
</tr>
<tr>
<td>lightcoral</td>
<td>240, 128, 128</td>
</tr>
<tr>
<td>lightcyan</td>
<td>224, 255, 255</td>
</tr>
<tr>
<td>lightgoldenrodyellow</td>
<td>250, 250, 210</td>
</tr>
<tr>
<td>lightgreen</td>
<td>144, 238, 145</td>
</tr>
<tr>
<td>lightgrey</td>
<td>211, 211, 211</td>
</tr>
<tr>
<td>lightpink</td>
<td>255, 182, 193</td>
</tr>
<tr>
<td>lightsalmon</td>
<td>255, 160, 122</td>
</tr>
<tr>
<td>lightsagegreen</td>
<td>32, 178, 170</td>
</tr>
<tr>
<td>lightskyblue</td>
<td>135, 206, 250</td>
</tr>
<tr>
<td>lightslategray</td>
<td>119, 136, 153</td>
</tr>
<tr>
<td>lightsteelblue</td>
<td>176, 196, 222</td>
</tr>
<tr>
<td>lightyellow</td>
<td>255, 255, 224</td>
</tr>
<tr>
<td>lime</td>
<td>0, 255, 0</td>
</tr>
<tr>
<td>limegreen</td>
<td>50, 205, 50</td>
</tr>
<tr>
<td>linen</td>
<td>250, 240, 230</td>
</tr>
<tr>
<td>magenta</td>
<td>255, 0, 255</td>
</tr>
<tr>
<td>maroon</td>
<td>128, 0, 0</td>
</tr>
<tr>
<td>mediumaquamarine</td>
<td>102, 205, 170</td>
</tr>
<tr>
<td>mediumblue</td>
<td>0, 0, 205</td>
</tr>
<tr>
<td>mediummorchid</td>
<td>186, 85, 211</td>
</tr>
<tr>
<td>mediumpurple</td>
<td>147, 112, 219</td>
</tr>
<tr>
<td>mediumseagreen</td>
<td>60, 179, 113</td>
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<tr>
<td>mediumslateblue</td>
<td>123, 104, 238</td>
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<tr>
<td>mediumsprinngreen</td>
<td>0, 250, 154</td>
</tr>
<tr>
<td>mediumturquoise</td>
<td>72, 209, 204</td>
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<tr>
<td>mediumvioletred</td>
<td>199, 21, 133</td>
</tr>
<tr>
<td>Midnightblue = 25, 25, 112</td>
<td>Mintcream = 245, 255, 250</td>
</tr>
<tr>
<td>--------------------------</td>
<td>--------------------------</td>
</tr>
<tr>
<td>Navy = 0, 0, 128</td>
<td>Oldlace = 253, 245, 230</td>
</tr>
<tr>
<td>Orangered = 255, 69, 0</td>
<td>Orchid = 218, 112, 214</td>
</tr>
<tr>
<td>Palevioletred = 219, 112, 147</td>
<td>Papayawhip = 255, 239, 213</td>
</tr>
<tr>
<td>Plum = 221, 160, 221</td>
<td>Powderblue = 176, 224, 230</td>
</tr>
<tr>
<td>Royalblue = 65, 105, 225</td>
<td>Saddlebrown = 139, 69, 19</td>
</tr>
<tr>
<td>Seashell = 255, 245, 238</td>
<td>Sienna = 160, 82, 45</td>
</tr>
<tr>
<td>Slategray = 112, 128, 144</td>
<td>Snow = 255, 250, 250</td>
</tr>
<tr>
<td>Teal = 0, 128, 128</td>
<td>Thistle = 216, 191, 216</td>
</tr>
<tr>
<td>Wheat = 245, 222, 179</td>
<td>White = 255, 255, 255</td>
</tr>
</tbody>
</table>

| Yellow = 255, 255, 0     | Yellowgreen = 154, 205, 50 |
dump molfile command

Syntax:

dump ID group-ID molfile N file format path

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be imaged
- molfile = style of dump command (other styles atom or cfg or dcd or xtc or xyz or local or custom are discussed on the dump doc page)
- N = dump every this many timesteps
- file = name of file to write to
- format = file format to be used
- path = file path with plugins (optional)

Examples:

dump mf1 all molfile 10 melt1.xml hoomd
dump mf2 all molfile 10 melt2-*.pdb pdb .
dump mf3 all molfile 50 melt3.xyz xyz .:/home/akohlmey/vmd/plugins/LINUX/molfile

Description:

Dump a snapshot of atom coordinates and selected additional quantities to one or more files every N timesteps in one of several formats. Only information for atoms in the specified group is dumped. This specific dump style uses molfile plugins that are bundled with the VMD molecular visualization and analysis program. See Section tools of the manual and the tools/lmp2vmd/README.txt file for more information about support in VMD for reading and visualizing native LAMMPS dump files.

Unless the filename contains a * character, the output will be written to one single file with the specified format. Otherwise there will be one file per snapshot and the * will be replaced by the time step number when the snapshot is written.

IMPORTANT NOTE: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom written to a dump file may be slightly outside the simulation box.

The molfile plugin API has a few restrictions that have to be honored by this dump style: the number of atoms must not change, the atoms must be sorted, outside of the coordinates no change in atom properties (like type, mass, charge) will be recorded.

The format keyword determines what format is used to write out the dump. For this to work, LAMMPS must be able to find and load a compatible molfile plugin that supports this format. Settings made via the dump_modify command can alter per atom properties like element names.

The path keyword determines which in directories. This is a "path" like other search paths, i.e. it can contain multiple directories separated by a colon (or semi-colon on windows). This keyword is optional and default to ".", the current directory.

The unwrap option of the dump_modify command allows coordinates to be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed through a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box.
Note that these coordinates may thus be far outside the box size stored with the snapshot.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the `dump_modify first` command, which can be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the `dump_modify every` command. The `dump_modify every` command also allows a variable to be used to determine the sequence of timesteps on which dump files are written.

**Restrictions:**

The `molfile` dump style is part of the USER-MOLFILE package. It is only enabled if LAMMPS was built with that package. See the **Making LAMMPS** section for more info.

Molfile plugins provide a consistent programming interface to read and write file formats commonly used in molecular simulations. The USER-MOLFILE package only provides the interface code, not the plugins. These can be obtained from a VMD installation which has to match the platform that you are using to compile LAMMPS for. By adding plugins to VMD, support for new file formats can be added to LAMMPS (or VMD or other programs that use them) without having to recompile the application itself. The plugins are installed in the directory: `/plugins/molfile`

NOTE: while the programming interface (API) to the plugins is backward compatible, the binary interface (ABI) has been changing over time, so it is necessary to compile this package with the plugin header files from VMD that match the binary plugins. These header files in the directory: `/plugins/include` For convenience, the package ships with a set of header files that are compatible with VMD 1.9 and 1.9.1 (June 2012)

**Related commands:**

`dump`, `dump_modify`, `undump`

**Default:**

The default path is ".". All other properties have to be specified.
**echo command**

**Syntax:**

`echo style`

- `style = none or screen or log or both`

**Examples:**

`echo both`
`echo log`

**Description:**

This command determines whether LAMMPS echoes each input script command to the screen and/or log file as it is read and processed. If an input script has errors, it can be useful to look at echoed output to see the last command processed.

The **command-line switch** `-echo` can be used in place of this command.

**Restrictions:** none

**Related commands:** none

**Default:**

`echo log`
fix command

Syntax:

fix ID group-ID style args

- ID = user-assigned name for the fix
- group-ID = ID of the group of atoms to apply the fix to
- style = one of a long list of possible style names (see below)
- args = arguments used by a particular style

Examples:

fix 1 all nve
fix 3 all nvt temp 300.0 300.0 0.01
fix mine top setforce 0.0 NULL 0.0

Description:

Set a fix that will be applied to a group of atoms. In LAMMPS, a "fix" is any operation that is applied to the system during timestepping or minimization. Examples include updating of atom positions and velocities due to time integration, controlling temperature, applying constraint forces to atoms, enforcing boundary conditions, computing diagnostics, etc. There are dozens of fixes defined in LAMMPS and new ones can be added; see this section for a discussion.

Fixes perform their operations at different stages of the timestep. If 2 or more fixes operate at the same stage of the timestep, they are invoked in the order they were specified in the input script.

The ID of a fix can only contain alphanumeric characters and underscores.

Fixes can be deleted with the unfix command.

IMPORTANT NOTE: The unfix command is the only way to turn off a fix; simply specifying a new fix with a similar style will not turn off the first one. This is especially important to realize for integration fixes. For example, using a fix nve command for a second run after using a fix nvt command for the first run, will not cancel out the NVT time integration invoked by the "fix nvt" command. Thus two time integrators would be in place!

If you specify a new fix with the same ID and style as an existing fix, the old fix is deleted and the new one is created (presumably with new settings). This is the same as if an "unfix" command were first performed on the old fix, except that the new fix is kept in the same order relative to the existing fixes as the old one originally was. Note that this operation also wipes out any additional changes made to the old fix via the fix_modify command.

The fix modify command allows settings for some fixes to be reset. See the doc page for individual fixes for details.

Some fixes store an internal "state" which is written to binary restart files via the restart or write_restart commands. This allows the fix to continue on with its calculations in a restarted simulation. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file. See the doc pages for individual fixes for info on which ones can be restarted.
Some fixes calculate one of three styles of quantities: global, per-atom, or local, which can be used by other commands or output as described below. A global quantity is one or more system-wide values, e.g. the energy of a wall interacting with particles. A per-atom quantity is one or more values per atom, e.g. the displacement vector for each atom since time 0. Per-atom values are set to 0.0 for atoms not in the specified fix group. Local quantities are calculated by each processor based on the atoms it owns, but there may be zero or more per atoms.

Note that a single fix may produces either global or per-atom or local quantities (or none at all), but never more than one of these.

Global, per-atom, and local quantities each come in three kinds: a single scalar value, a vector of values, or a 2d array of values. The doc page for each fix describes the style and kind of values it produces, e.g. a per-atom vector. Some fixes produce more than one kind of a single style, e.g. a global scalar and a global vector.

When a fix quantity is accessed, as in many of the output commands discussed below, it can be referenced via the following bracket notation, where ID is the ID of the fix:

- \[ f_{\text{ID}} \] entire scalar, vector, or array
- \[ f_{\text{ID}}[i] \] one element of vector, one column of array
- \[ f_{\text{ID}}[i][j] \] one element of array

In other words, using one bracket reduces the dimension of the quantity once (vector -> scalar, array -> vector). Using two brackets reduces the dimension twice (array -> scalar). Thus a command that uses scalar fix values as input can also process elements of a vector or array.

Note that commands and variables which use fix quantities typically do not allow for all kinds, e.g. a command may require a vector of values, not a scalar. This means there is no ambiguity about referring to a fix quantity as \[ f_{\text{ID}} \] even if it produces, for example, both a scalar and vector. The doc pages for various commands explain the details.

In LAMMPS, the values generated by a fix can be used in several ways:

- Global values can be output via the thermo_style custom or fix ave/time command. Or the values can be referenced in a variable equal or variable atom command.
- Per-atom values can be output via the dump custom command or the fix ave/spatial command. Or they can be time-averaged via the fix ave/atom command or reduced by the compute reduce command. Or the per-atom values can be referenced in an atom-style variable.
- Local values can be reduced by the compute reduce command, or histogrammed by the fix ave/histo command.

See this howto section for a summary of various LAMMPS output options, many of which involve fixes.

The results of fixes that calculate global quantities can be either "intensive" or "extensive" values. Intensive means the value is independent of the number of atoms in the simulation, e.g. temperature. Extensive means the value scales with the number of atoms in the simulation, e.g. total rotational kinetic energy. Thermodynamic output will normalize extensive values by the number of atoms in the system, depending on the "thermo_modify norm" setting. It will not normalize intensive values. If a fix value is accessed in another way, e.g. by a variable, you may want to know whether it is an intensive or extensive value. See the doc page for individual fixes for further info.

Each fix style has its own documentation page which describes its arguments and what it does, as listed below.

Here is an alphabetic list of fix styles available in LAMMPS:
- adapt - change a simulation parameter over time
- addforce - add a force to each atom
- append/atoms - append atoms to a running simulation
- aveforce - add an averaged force to each atom
- ave/atom - compute per-atom time-averaged quantities
- ave/histo - compute/output time-averaged histograms
- ave/spatial - compute/output time-averaged per-atom quantities by layer
- ave/time - compute/output global time-averaged quantities
- bond/break - break bonds on the fly
- bond/create - create bonds on the fly
- bond/swap - Monte Carlo bond swapping
- box/relax - relax box size during energy minimization
- deform - change the simulation box size/shape
- deposit - add new atoms above a surface
- drag - drag atoms towards a defined coordinate
- dt/reset - reset the timestep based on velocity, forces
- efield - impose electric field on system
- enforce2d - zero out z-dimension velocity and force
- evaporate - remove atoms from simulation periodically
- external - callback to an external driver program
- freeze - freeze atoms in a granular simulation
- gravity - add gravity to atoms in a granular simulation
- gcme - grand canonical insertions/deletions
- heat - add/subtract momentum-conserving heat
- indent - impose force due to an indenter
- langevin - Langevin temperature control
- lineforce - constrain atoms to move in a line
- momentum - zero the linear and/or angular momentum of a group of atoms
- move - move atoms in a prescribed fashion
- msst - multi-scale shock technique (MSST) integration
- neb - nudged elastic band (NEB) spring forces
- nph - constant NPH time integration via Nose/Hoover
- nph/asphere - NPH for aspherical particles
- nph/sphere - NPH for spherical particles
- nphug - constant-stress Hugoniostat integration
- npt - constant NPT time integration via Nose/Hoover
- npt/asphere - NPT for aspherical particles
- npt/sphere - NPT for spherical particles
- nve - constant NVE time integration
- nve/asphere - NVE for aspherical particles
- nve/asphere/noforce - NVE for aspherical particles without forces
- nve/limit - NVE with limited step length
- nve/line - NVE for line segments
- nve/noforce - NVE without forces (v only)
- nve/sphere - NVE for spherical particles
- nve/tri - NVE for triangles
- nvt - constant NVT time integration via Nose/Hoover
- nvt/asphere - NVT for aspherical particles
- nvt/sllod - NVT for NEMD with SLLOD equations
- nvt/sphere - NVT for spherical particles
- orient/fcc - add grain boundary migration force
- planeforce - constrain atoms to move in a plane
• poems - constrain clusters of atoms to move as coupled rigid bodies
• pour - pour new atoms into a granular simulation domain
• press/berendsen - pressure control by Berendsen barostat
• print - print text and variables during a simulation
• reax/bonds - write out ReaxFF bond information recenter - constrain the center-of-mass position of a group of atoms
• restrain - constrain a bond, angle, dihedral
• rigid - constrain one or more clusters of atoms to move as a rigid body with NVE integration
• rigid/nph - constrain one or more clusters of atoms to move as a rigid body with NPH integration
• rigid/npt - constrain one or more clusters of atoms to move as a rigid body with NPT integration
• rigid/nve - constrain one or more clusters of atoms to move as a rigid body with alternate NVE integration
• rigid/nvt - constrain one or more clusters of atoms to move as a rigid body with NVT integration
• setforce - set the force on each atom
• shake - SHAKE constraints on bonds and/or angles
• spring - apply harmonic spring force to group of atoms
• spring/rg - spring on radius of gyration of group of atoms
• spring/self - spring from each atom to its origin
• srd - stochastic rotation dynamics (SRD)
• store/force - store force on each atom
• store/state - store attributes for each atom
• temp/berendsen - temperature control by Berendsen thermostat
• temp/rescale - temperature control by velocity rescaling
• thermal/conductivity - Muller-Plathe kinetic energy exchange for thermal conductivity calculation
• tmd - guide a group of atoms to a new configuration
• ttm - two-temperature model for electronic/atomic coupling
• viscosity - Muller-Plathe momentum exchange for viscosity calculation
• viscous - viscous damping for granular simulations
• wall/colloid - Lennard-Jones wall interacting with finite-size particles
• wall/gra - frictional wall(s) for granular simulations
• wall/harmonic - harmonic spring wall
• wall/lj126 - Lennard-Jones 12-6 wall
• wall/lj93 - Lennard-Jones 9-3 wall
• wall/piston - moving reflective piston wall
• wall/reflect - reflecting wall(s)
• wall/region - use region surface as wall
• wall/srd - slip/no-slip wall for SRD particles

There are also additional fix styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the fix section of this page.

There are also additional accelerated fix styles included in the LAMMPS distribution for faster performance on CPUs and GPUs. The list of these with links to the individual styles are given in the pair section of this page.

Restrictions:

Some fix styles are part of specific packages. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual fixes tell if it is part of a package.

Related commands:

unfix, fix_modify
Default: none
fix adapt command

Syntax:

fix ID group-ID adapt N attribute args ... keyword value ...

- ID, group-ID are documented in fix command
- adapt = style name of this fix command
- N = adapt simulation settings every this many timesteps
- one or more attribute/arg pairs may be appended
- attribute = pair or kspace or atom

pair args = pstyle pparam I J v_name
  pstyle = pair style name, e.g. lj/cut
  pparam = parameter to adapt over time
  I, J = type pair(s) to set parameter for
  v_name = variable with name that calculates value of pparam

kspace arg = v_name
  v_name = variable with name that calculates scale factor on K-space terms

atom args = aparam v_name
  aparam = parameter to adapt over time
  v_name = variable with name that calculates value of aparam

- zero or more keyword/value pairs may be appended
- keyword = scale or reset

scale value = no or yes
  no = the variable value is the new setting
  yes = the variable value multiplies the original setting

reset value = no or yes
  no = values will remain altered at the end of a run
  yes = reset altered values to their original values at the end of a run

Examples:

fix 1 all adapt 1 pair soft a 1 1 v_prefactor
fix 1 all adapt 1 pair soft a 2* 3 v_prefactor
fix 1 all adapt 1 pair lj/cut epsilon * * v_scale1 coul/cut scale 3 3 v_scale2 scale yes reset yes
fix 1 all adapt 10 atom diameter v_size

Description:

Change or adapt one or more specific simulation attributes or settings over time as a simulation runs. Pair potential and K-space and atom attributes which can be varied by this fix are discussed below. Many other fixes can also be used to time-vary simulation parameters, e.g. the "fix deform" command will change the simulation box size/shape and the "fix move" command will change atom positions and velocities in a prescribed manner.

If N is specified as 0, the specified attributes are only changed once, before the simulation begins. This is all that is needed if the associated variables are not time-dependent. If N > 0, then changes are made every N steps during the simulation, presumably with a variable that is time-dependent.

Depending on the value of the reset keyword, attributes changed by this fix will or will not be reset back to their original values at the end of a simulation. Even if reset is specified as yes, a restart file written during a simulation will contain the modified settings.
IMPORTANT NOTE: Currently, only the pair and kspace params are resetable. Atom attributes are not. This will be added at some point.

If the scale keyword is set to no, then the value the parameter is set to will be whatever the variable generates. If the scale keyword is set to yes, then the value of the altered parameter will be the initial value of that parameter multiplied by whatever the variable generates. I.e. the variable is now a "scale factor" applied in (presumably) a time-varying fashion to the parameter. Internally, the parameters themselves are actually altered; make sure you use the reset yes option if you want the parameters to be restored to their initial values after the run.

The pair keyword enables various parameters of potentials defined by the pair_style command to be changed, if the pair style supports it. Note that the pair_style and pair_coeff commands must be used in the usual manner to specify these parameters initially; the fix adapt command simply overrides the parameters.

The pstyle argument is the name of the pair style. If pair_style hybrid or hybrid/overlay is used, pstyle should be a sub-style name. For example, pstyle could be specified as "soft" or "lubricate". The pparam argument is the name of the parameter to change. This is the current list of pair styles and parameters that can be varied by this fix. See the doc pages for individual pair styles and their energy formulas for the meaning of these parameters:

<table>
<thead>
<tr>
<th>pstyle</th>
<th>pparam</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>born</td>
<td>a,b,c</td>
<td>type pairs</td>
</tr>
<tr>
<td>buck</td>
<td>a,c</td>
<td>type pairs</td>
</tr>
<tr>
<td>coul/cut</td>
<td>scale</td>
<td>type pairs</td>
</tr>
<tr>
<td>coul/debye</td>
<td>scale</td>
<td>type pairs</td>
</tr>
<tr>
<td>coul/long</td>
<td>scale</td>
<td>type pairs</td>
</tr>
<tr>
<td>lj/cut</td>
<td>epsilon</td>
<td>type pairs</td>
</tr>
<tr>
<td>lj/cut/opt</td>
<td>epsilon</td>
<td>type pairs</td>
</tr>
<tr>
<td>lubricate</td>
<td>mu</td>
<td>global</td>
</tr>
<tr>
<td>gauss</td>
<td>a</td>
<td>type pairs</td>
</tr>
<tr>
<td>soft</td>
<td>a</td>
<td>type pairs</td>
</tr>
</tbody>
</table>

IMPORTANT NOTE: It is easy to add new potentials and their parameters to this list. All it typically takes is adding an extract() method to the pair_*.cpp file associated with the potential.

Some parameters are global settings for the pair style, e.g. the viscosity setting "mu" for pair_style lubricate. Other parameters apply to atom type pairs within the pair style, e.g. the prefactor "a" for pair_style soft.

Note that for many of the potentials, the parameter that can be varied is effectively a prefactor on the entire energy expression for the potential, e.g. the lj/cut epsilon. The parameters listed as "scale" are exactly that, since the energy expression for the coul/cut potential (for example) has no labeled prefactor in its formula. To apply an effective prefactor to some potentials, multiple parameters need to be altered. For example, the Buckingham potential needs both the A and C terms altered together. To scale the Buckingham potential, you should thus list the pair style twice, once for A and once for C.

If a type pair parameter is specified, the I and J settings should be specified to indicate which type pairs to apply it to. If a global parameter is specified, the I and J settings still need to be specified, but are ignored.

Similar to the pair_coeff command, I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values.

A wild-card asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types,
then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

IMPORTANT NOTE: If pair_style hybrid or hybrid/overlay is being used, then the pstyle will be a sub-style name. You must specify I,J arguments that correspond to type pair values defined (via the pair_coeff command) for that sub-style.

The v_name argument for keyword pair is the name of an equal-style variable which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable name. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify parameters that change as a function of time or span consecutive runs in a continuous fashion. For the latter, see the start and stop keywords of the run command and the elaplong keyword of thermo_style custom for details.

For example, these commands would change the prefactor coefficient of the pair_style soft potential from 10.0 to 30.0 in a linear fashion over the course of a simulation:

```
variable prefactor equal ramp(10,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

The kspace keyword used the specified variable as a scale factor on the energy, forces, virial calculated by whatever K-Space solver is defined by the kspace_style command. If the variable has a value of 1.0, then the solver is unaltered.

The kspace keyword works this way whether the scale keyword is set to no or yes.

The atom keyword enables various atom properties to be changed. The aparam argument is the name of the parameter to change. This is the current list of atom parameters that can be varied by this fix:

- diameter = diameter of particle

The v_name argument of the atom keyword is the name of an equal-style variable which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable name. See the discussion above describing the formulas associated with equal-style variables. The new value is assigned to the corresponding attribute for all atoms in the fix group.

If the atom parameter is diameter and per-atom density and per-atom mass are defined for particles (e.g. atom_style granular), then the mass of each particle is also changed when the diameter changes (density is assumed to stay constant).

For example, these commands would shrink the diameter of all granular particles in the "center" group from 1.0 to 0.1 in a linear fashion over the course of a 1000-step simulation:

```
variable size equal ramp(1.0,0.1)
fix 1 center adapt 10 atom diameter v_size
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter
of this fix can be used with the \textit{start/stop} keywords of the \texttt{run} command. This fix is not invoked during \texttt{energy minimization}.

\textbf{Restrictions:} none

\textbf{Related commands:}

\texttt{compute ti}

\textbf{Default:}

The option defaults are scale = no, reset = no.
fix addforce command

fix addforce/cuda command

Syntax:

fix ID group-ID addforce fx fy fz keyword value ...

• ID, group-ID are documented in fix command
• addforce = style name of this fix command
• fx,fy,fz = force component values (force units)

  any of fx,fy,fz can be a variable (see below)

• zero or more keyword/value pairs may be appended to args
• keyword = region or energy

  region value = region-ID
    region-ID = ID of region atoms must be in to have added force
  energy value = v_name
    v_name = variable with name that calculates the potential energy of each atom in the added force

Examples:

fix kick flow addforce 1.0 0.0 0.0
fix kick flow addforce 1.0 0.0 v_oscillate
fix ff boundary addforce 0.0 0.0 v_push energy v_espace

Description:

Add fx,fy,fz to the corresponding component of force for each atom in the group. This command can be used to
give an additional push to atoms in a simulation, such as for a simulation of Poiseuille flow in a channel.

Any of the 3 quantities defining the force components can be specified as an equal-style or atom-style variable,

namely fx,fy,fz. If the value is a variable, it should be specified as v_name, where name is the variable name. In

this case, the variable will be evaluated each timestep, and its value used to determine the force component.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style

command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a
time-dependent force field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values,

such as atom coordinates. Thus it is easy to specify a spatially-dependent force field with optional
time-dependence as well.

If the region keyword is used, the atom must also be in the specified geometric region in order to have force

added to it.

Adding a force to atoms implies a change in their potential energy as they move due to the applied force field. For
dynamics via the "run" command, this energy can be optionally added to the system's potential energy for

thermodynamic output (see below). For energy minimization via the "minimize" command, this energy must be

added to the system's potential energy to formulate a self-consistent minimization problem (see below).
The energy keyword is not allowed if the added force is a constant vector $F = (f_x, f_y, f_z)$, with all components defined as numeric constants and not as variables. This is because LAMMPS can compute the energy for each atom directly as $E = -x \cdot F = -(x*f_x + y*f_y + z*f_z)$, so that $-\text{Grad}(E) = F$.

The energy keyword is optional if the added force is defined with one or more variables, and if you are performing dynamics via the run command. If the keyword is not used, LAMMPS will set the energy to 0.0, which is typically fine for dynamics.

The energy keyword is required if the added force is defined with one or more variables, and you are performing energy minimization via the "minimize" command. The keyword specifies the name of an atom-style variable which is used to compute the energy of each atom as function of its position. Like variables used for $f_x$, $f_y$, $f_z$, the energy variable is specified as $v_name$, where name is the variable name.

Note that when the energy keyword is used during an energy minimization, you must insure that the formula defined for the atom-style variable is consistent with the force variable formulas, i.e. that $-\text{Grad}(E) = F$. For example, if the force were a spring-like $F = kx$, then the energy formula should be $E = -0.5kx^2$. If you don't do this correctly, the minimization will not converge properly.

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify energy option is supported by this fix to add the potential "energy" inferred by the added force to the system's potential energy as part of thermodynamic output. This is a fictitious quantity but is needed so that the minimize command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added force.

This fix computes a global scalar and a global 3-vector of forces, which can be accessed by various output commands. The scalar is the potential energy discussed above. The vector is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. You should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.
IMPORTANT NOTE: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the `fix_modify energy` option for this fix.

Restrictions: none

Related commands:

fix setforce, fix aveforce

Default: none
fix addtorque command

Syntax:

fix ID group-ID addtorque Tx Ty Tz

- ID, group-ID are documented in fix command
- addtorque = style name of this fix command
- Tx, Ty, Tz = torque component values (torque units)
- any of Tx, Ty, Tz can be a variable (see below)

Examples:

fix kick bead addtorque 2.0 3.0 5.0
fix kick bead addtorque 0.0 0.0 v_oscillate

Description:

Add a set of forces to each atom in the group such that:

- the components of the total torque applied on the group (around its center of mass) are Tx, Ty, Tz
- the group would move as a rigid body in the absence of other forces.

This command can be used to drive a group of atoms into rotation.

Any of the 3 quantities defining the torque components can be specified as an equal-style variable, namely Tx, Ty, Tz. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the torque component.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent torque.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify energy option is supported by this fix to add the potential "energy" inferred by the added forces to the system's potential energy as part of thermodynamic output. This is a fictitious quantity but is needed so that the minimize command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added forces.

This fix computes a global scalar and a global 3-vector, which can be accessed by various output commands. The scalar is the potential energy discussed above. The vector is the total torque on the group of atoms before the forces on individual atoms are changed by the fix. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. You
should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

**Restrictions:**

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the [Making LAMMPS](#) section for more info.

**Related commands:**

fix addforce

**Default:** none
fix append/atoms command

Syntax:

fix ID group-ID append/atoms face ... keyword value ...

- ID, group-ID are documented in fix command
- append/atoms = style name of this fix command
- face = zhi
- zero or more keyword/value pairs may be appended
- keyword = size or freq or temp or random or units

size args = Lz
  Lz = z size of lattice region appended in a single event (distance units)
freq args = freq
  freq = the number of timesteps between append events
temp args = target damp seed extent
  target = target velocity for region immediately ahead of the piston
  damp = damping parameter (time units)
  seed = random number seed for langevin kicks
  extent = extent of thermostated region (distance units)
random args = xmax ymax zmax seed
  xmax, ymax, zmax = maximum displacement in particular direction (distance units)
  seed = random number seed for random displacement
units value = lattice or box
  lattice = the wall position is defined in lattice units
  box = the wall position is defined in simulation box units

Examples:

fix 1 all append/atoms zhi size 5.0 freq 295 units lattice
fix 4 all append/atoms zhi size 15.0 freq 5 units box
fix A all append/atoms zhi size 1.0 freq 1000 units lattice

Description:

This fix creates atoms on a lattice, appended on the zhi edge of the system box. This can be useful when a shock or wave is propagating from zlo. This allows the system to grow with time to accommodate an expanding wave. A simulation box must already exist, which is typically created via the create_box command. Before using this command, a lattice must also be defined using the lattice command.

This fix will automatically freeze atoms on the zhi edge of the system, so that overlaps are avoided when new atoms are appended.

The size keyword defines the size in z of the chunk of material to be added.

The random keyword will give the atoms random displacements around their lattice points to simulate some initial temperature.

The temp keyword will cause a region to be thermostated with a Langevin thermostat on the zhi boundary. The size of the region is measured from zhi and is set with the extent argument.

The units keyword determines the meaning of the distance units used to define a wall position, but only when a
numeric constant is used. A box value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A lattice value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacings.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The boundary on which atoms are added with append/atoms must be shrink/minimum. The opposite boundary may be any boundary type other than periodic.

**Related commands:**

fix wall/piston command

**Default:**

The keyword defaults are size = 0.0, freq = 0, units = lattice.
fix atc command

Syntax:

fix ID groupID atc type paramfile

• ID, group-ID are documented in fix command
• atc = style name of this fix command
• type = thermal or two_temperature or hardy

thermal = thermal coupling with field: temperature
two_temperature = electron-phonon coupling with field, temperature and electron_temperature
hardy = Hardy on-the-fly post-processing

• paramfile = file with material parameters (not specified for hardy type)

Examples:

fix AtC atc_atoms atc thermal Ar_thermal.dat
fix AtC atc_atoms atc transfer hardy

Description:

This fix creates a coupled finite element (FE) and molecular dynamics (MD) simulation and/or an on-the-fly estimation of continuum fields, where a FE mesh is specified and overlaps the particles, something like this:

Interscale operators are defined that construct continuum fields from atomic data. Coupled simulations use FE projection approximated on a discrete field. Currently, coupling is restricted to thermal physics. The Hardy module can use either FE projection or integration Kernels evaluated at mesh points.

Coupling methods enable appropriate corrections to the atomic data to be made based on the FE field. For example, a Gaussian isokinetic thermostat can apply heat sources to the atoms that varies in space on the same scale as the FE element size. Meshes are not created automatically and must be specified on LAMMPS regions with prescribed element sizes.

Coupling and post-processing can be combined in the same simulations using separate fix atc commands.

Note that mesh computations and storage run in serial (not parallelized) so performance will degrade when large element counts are used.
For detailed exposition of the theory and algorithms implemented in this fix, please see the papers here and here. Please refer to the standard finite element (FE) texts, such as this book, for the basics of FE simulation.

*Thermal* and *two_temperature* (coupling) types use a Verlet time-integration algorithm. The *hardy* type does not contain its own time-integrator and must be used with a separate fix that does contain one, e.g. fix nve, fix nvt, etc.

A set of example input files with the attendant material files are included in the examples/USER/atc directory of the LAMMPS distribution.

An extensive set of additional documentation pages for the options turned on via the fix_modify command for this fix are included in the doc/USER/atc directory of the LAMMPS distribution. Individual doc pages are listed and linked to below.

The following commands are typical of a coupling problem:

```plaintext
# ... commands to create and initialize the MD system

# initial fix to designate coupling type and group to apply it to
# tag group physics material_file
fix AtC internal atc thermal Ar_thermal.mat

# create a uniform 12 x 2 x 2 mesh that covers region contain the group
# nx ny nz region periodicity
fix_modify AtC fem create mesh 12 2 2 mdRegion f p p

# specify the control method for the type of coupling
# physics control_type
fix_modify AtC transfer thermal control flux

# specify the initial values for the empirical field "temperature"
# field node_group value
fix_modify AtC transfer initial temperature all 30.0

# create an output stream for nodal fields
# filename output_frequency
fix_modify AtC transfer output atc_fe_output 100

run 1000
```

The following commands are typical of a post-processing (Hardy) problem:

```plaintext
# ... commands to create and initialize the MD system

# initial fix to designate post-processing and the group to apply it to
# no material file is allowed nor required
fix AtC internal atc hardy

# create a uniform 1 x 1 x 1 mesh that covers region contain the group
# with periodicity this effectively creates a system average
fix_modify AtC fem create mesh 1 1 1 box p p p

# change from default lagrangian map to eulerian
# refreshed every 100 steps
fix_modify AtC atom_element_map eulerian 100

# start with no field defined
fix_modify AtC transfer fields none
```
[72x747]# add mass density, potential energy density, stress and temperature
fix_modify AtC transfer fields add density energy stress temperature

# create an output stream for nodal fields
# filename output_frequency
fix_modify AtC transfer output nvtFE 100 text

run 1000

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. The fix_modify options relevant to this fix are listed below. No global scalar or vector or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-ATC package. It is only enabled if LAMMPS was built with that package, which also requires the ATC library be built and linked with LAMMPS. See the Making LAMMPS section for more info.

Related commands:

After specifying this fix in your input script, several other fix_modify commands are used to setup the problem, e.g. define the finite element mesh and prescribe initial and boundary conditions.

fix_modify commands for setup:

- fix_modify AtC fem create mesh
- fix_modify AtC mesh create_nodeset
- fix_modify AtC mesh create_faceset
- fix_modify AtC mesh create_elementset
- fix_modify AtC transfer internal
- fix_modify AtC transfer boundary
- fix_modify AtC transfer internal_quadrature
- fix_modify AtC transfer pmfc
- fix_modify AtC extrinsic electron_integration

fix_modify commands for boundary and initial conditions:

- fix_modify AtC transfer initial
- fix_modify AtC transfer fix
- fix_modify AtC transfer unfix
- fix_modify AtC transfer fix_flux
- fix_modify AtC transfer_unfix_flux
- fix_modify AtC transfer source
- fix_modify AtC transfer remove_source

fix_modify commands for control and filtering:

- fix_modify AtC transfer thermal control
- fix_modify AtC transfer filter
• fix_modify AtC transfer filter scale
• fix_modify AtC transfer equilibrium_start
• fix_modify AtC extrinsic exchange

fix_modify commands for output:

• fix_modify AtC transfer output
• fix_modify AtC transfer atomic_output
• fix_modify AtC mesh output
• fix_modify AtC transfer write_restart
• fix_modify AtC transfer read_restart

fix_modify commands for post-processing:

• fix_modify AtC transfer fields
• fix_modify AtC transfer gradients
• fix_modify AtC transfer rates
• fix_modify AtC transfer computes
• fix_modify AtC set
• fix_modify AtC transfer on_the_fly
• fix_modify AtC boundary_integral
• fix_modify AtC contour_integral

miscellaneous fix_modify commands:

• fix_modify AtC transfer atom_element_map
• fix_modify AtC transfer neighbor_reset_frequency

Default: none

---


(Zimmerman) Zimmerman, Webb, Hoyt, Jones, Klein, Bammann, Special Issue of Modelling and Simulation in Materials Science and Engineering, 12, S319 (2004).

fix ave/atom command

Syntax:

fix ID group-ID ave/atom Nevery Nrepeat Nfreq value1 value2 ...  

- ID, group-ID are documented in fix command
- ave/atom = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps one or more input values can be listed
- value = x, y, z, vx, vy, vz, fx, fy, fz, c_ID, c_ID[i], f_ID, f_ID[i], v_name
  - x, y, z, vx, vy, vz = atom attribute (position, velocity, force component)
  - c_ID = per-atom vector calculated by a compute with ID
  - c_ID[i] = Ith column of per-atom array calculated by a compute with ID
  - f_ID = per-atom vector calculated by a fix with ID
  - f_ID[i] = Ith column of per-atom array calculated by a fix with ID
  - v_name = per-atom vector calculated by an atom-style variable with name

Examples:

fix 1 all ave/atom 1 100 100 vx vy vz
fix 1 all ave/atom 10 20 1000 c_my_stress[1]

Description:

Use one or more per-atom vectors as inputs every few timesteps, and average them atom by atom over longer timescales. The resulting per-atom averages can be used by other output commands such as the fix ave/spatial or dump custom commands.

The group specified with the command means only atoms within the group have their averages computed. Results are set to 0.0 for atoms not in the group.

Each input value can be an atom attribute (position, velocity, force component) or can be the result of a compute or fix or the evaluation of an atom-style variable. In the latter cases, the compute, fix, or variable must produce a per-atom vector, not a global quantity or local quantity. If you wish to time-average global quantities from a compute, fix, or variable, then see the fix ave/time command.

Computes that produce per-atom vectors or arrays are those which have the word atom in their style name. See the doc pages for individual fixes to determine which ones produce per-atom vectors or arrays. Variables of style atom are the only ones that can be used with this fix since they produce per-atom vectors.

Each per-atom value of each input vector is averaged independently.

The Nevery, Nrepeat, and Nfreq arguments specify on what timesteps the input values will be used in order to contribute to the average. The final averaged quantities are generated on timesteps that are a multiple of Nfreq. The average is over Nrepeat quantities, computed in the preceding portion of the simulation every Nevery timesteps. Nfreq must be a multiple of Nevery and Nevery must be non-zero even if Nrepeat is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nfreq > (Nrepeat-1)*Nevery is required.
For example, if \( Nevery=2 \), \( Nrepeat=6 \), and \( Nfreq=100 \), then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc.

The atom attribute values \((x,y,z,vx,vy,vz,fx,fy,fz)\) are self-explanatory. Note that other atom attributes can be used as inputs to this fix by using the \texttt{compute property/atom} command and then specifying an input value from that compute.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed term is appended, the per-atom vector calculated by the compute is used. If a bracketed term containing an index \( I \) is appended, the \( I \)th column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and \texttt{add them to LAMMPS}.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed term is appended, the per-atom vector calculated by the fix is used. If a bracketed term containing an index \( I \) is appended, the \( I \)th column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with \( Nevery \), else an error will result. Users can also write code for their own fix styles and \texttt{add them to LAMMPS}.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script as an \texttt{atom-style variable} Variables of style \texttt{atom} can reference thermodynamic keywords, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to time average.

\textbf{Restart, fix\_modify, output, run start/stop, minimize info:}

No information about this fix is written to binary restart files. None of the \texttt{fix\_modify} options are relevant to this fix. No global scalar or vector quantities are stored by this fix for access by various \texttt{output commands}.

This fix produces a per-atom vector or array which can be accessed by various \texttt{output commands}. A vector is produced if only a single quantity is averaged by this fix. If two or more quantities are averaged, then an array of values is produced. The per-atom values can only be accessed on timesteps that are multiples of \( Nfreq \) since that is when averaging is performed.

No parameter of this fix can be used with the \texttt{start/stop} keywords of the \texttt{run} command. This fix is not invoked during energy minimization.

\textbf{Restrictions:} none

\textbf{Related commands:}

\texttt{compute, fix ave/histo, fix ave/spatial, fix ave/time, variable,}

\textbf{Default:} none
fix ave/correlate command

Syntax:

```
fix ID group-ID ave/correlate Nevery Nrepeat Nfreq value1 value2 ... keyword args ...
```

- ID, group-ID are documented in fix command
- ave/correlate = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of correlation time windows to accumulate
- Nfreq = calculate time window averages every this many timesteps
- one or more input values can be listed
- value = c_ID, c_ID[N], f_ID, f_ID[N], v_name
  - c_ID = global scalar calculated by a compute with ID
  - c_ID[I] = Ith component of global vector calculated by a compute with ID
  - f_ID = global scalar calculated by a fix with ID
  - f_ID[I] = Ith component of global vector calculated by a fix with ID
  - v_name = global value calculated by an equal-style variable with name
- zero or more keyword/arg pairs may be appended
- keyword = type or ave or start or prefactor or file or overwrite or title1 or title2 or title3

  - type arg = auto or upper or lower or auto/upper or auto/lower or full
    - auto = correlate each value with itself
    - upper = correlate each value with each succeeding value
    - lower = correlate each value with each preceding value
    - auto/upper = auto + upper
    - auto/lower = auto + lower
    - full = correlate each value with every other value, including itself = auto + upper + lower
  - ave args = one or running
    - one = zero the correlation accumulation every Nfreq steps
    - running = accumulate correlations continuously
  - start args = Nstart
    - Nstart = start accumulating correlations on this timestep
  - prefactor args = value
    - value = prefactor to scale all the correlation data by
  - file arg = filename
    - filename = name of file to output correlation data to
  - overwrite arg = none = overwrite output file with only latest output
  - title1 arg = string
    - string = text to print as 1st line of output file
  - title2 arg = string
    - string = text to print as 2nd line of output file
  - title3 arg = string
    - string = text to print as 3rd line of output file

Examples:

```
fix 1 all ave/correlate 5 100 1000 c_myTemp file temp.correlate
fix 1 all ave/correlate 1 50 10000 &
  type upper ave running title1 "My correlation data"
```

Description:
Use one or more global scalar values as inputs every few timesteps, calculate time correlations between them at varying time intervals, and average the correlation data over longer timescales. The resulting correlation values can be time integrated by variables or used by other output commands such as thermo_style custom, and can also be written to a file.

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a compute or fix or the evaluation of an equal-style variable. In each case, the compute, fix, or variable must produce a global quantity, not a per-atom or local quantity. If you wish to spatial- or time-average or histogram per-atom quantities from a compute, fix, or variable, then see the fix ave/spatial, fix ave/atom, or fix ave/histo commands. If you wish to sum a per-atom quantity into a single global quantity, see the compute reduce command.

Computes that produce global quantities are those which do not have the word atom in their style name. Only a few fixes produce global quantities. See the doc pages for individual fixes for info on which ones produce such values. Variables of style equal are the only ones that can be used with this fix. Variables of style atom cannot be used, since they produce per-atom values.

The input values must either be all scalars. What kinds of correlations between input values are calculated is determined by the type keyword as discussed below.

The Nevery, Nrepeat, and Nfreq arguments specify on what timesteps the input values will be used to calculate correlation data. The input values are sampled every Nevery timesteps. The correlation data for the preceding samples is computed on timesteps that are a multiple of Nfreq. Consider a set of samples from some initial time up to an output timestep. The initial time could be the beginning of the simulation or the last output time; see the ave keyword for options. For the set of samples, the correlation value Cij is calculated as:

\[ C_{ij}(\delta) = \text{ave}(V_i(t) \times V_j(t+\delta)) \]

which is the correlation value between input values Vi and Vj, separated by time delta. Note that the second value Vj in the pair is always the one sampled at the later time. The ave() represents an average over every pair of samples in the set that are separated by time delta. The maximum delta used is of size \((N\text{repeat}-1)\times\text{Nevery}\). Thus the correlation between a pair of input values yields Nrepeat correlation datums:

\[ C_{ij}(0), C_{ij}(\text{Nevery}), C_{ij}(2\times\text{Nevery}), \ldots, C_{ij}((N\text{repeat}-1)\times\text{Nevery}) \]

For example, if Nevery=5, Nrepeat=6, and Nfreq=100, then values on timesteps 0,5,10,15,...,100 will be used to compute the final averages on timestep 100. Six averages will be computed: Cij(0), Cij(5), Cij(10), Cij(15), Cij(20), and Cij(25). Cij(10) on timestep 100 will be the average of 19 samples, namely Vi(0)\times Vj(10), Vi(5)\times Vj(15), Vi(10)\times Vj(20), Vi(15)\times Vj(25), ..., Vi(85)\times Vj(95), Vi(90)\times Vj(100).

Nfreq must be a multiple of Nevery; Nevery and Nrepeat must be non-zero. Also, if the ave keyword is set to one which is the default, then Nfreq >= (Nrepeat-1)\times Nevery is required.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used.

Note that there is a compute reduce command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix ave/correlate. Or it can be a compute defined not in your input script, but by thermodynamic output or other fixes such as fix nvt or fix temp/rescale. See the doc pages for these commands.
which give the IDs of these computes. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used.

Note that some fixes only produce their values on certain timesteps, which must be compatible with Nevery, else an error will result. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Only equal-style variables can be referenced. See the variable command for details. Note that variables of style equal define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to time correlate.

Additional optional keywords also affect the operation of this fix.

The type keyword determines which pairs of input values are correlated with each other. For N input values Vi, for i = 1 to N, let the number of pairs = Npair. Note that the second value in the pair Vi(t)*Vj(t+delta) is always the one sampled at the later time.

- If type is set to auto then each input value is correlated with itself. I.e. Cii = Vi*Vi, for i = 1 to N, so Npair = N.
- If type is set to upper then each input value is correlated with every succeeding value. I.e. Cij = Vi*Vj, for i < j, so Npair = N*(N-1)/2.
- If type is set to lower then each input value is correlated with every preceding value. I.e. Cij = Vi*Vj, for i > j, so Npair = N*(N-1)/2.
- If type is set to auto/upper then each input value is correlated with itself and every succeeding value. I.e. Cij = Vi*Vj, for i >= j, so Npair = N*(N+1)/2.
- If type is set to auto/lower then each input value is correlated with itself and every preceding value. I.e. Cij = Vi*Vj, for i <= j, so Npair = N*(N+1)/2.
- If type is set to full then each input value is correlated with itself and every other value. I.e. Cij = Vi*Vj, for i,j = 1,N so Npair = N^2.

The ave keyword determines what happens to the accumulation of correlation samples every Nfreq timesteps. If the ave setting is one, then the accumulation is restarted or zeroed every Nfreq timesteps. Thus the outputs on successive Nfreq timesteps are essentially independent of each other. The exception is that the Cij(0) = Vi(T)*Vj(T) value at a timestep T, where T is a multiple of Nfreq, contributes to the correlation output both at time T and at time T+Nfreq.

If the ave setting is running, then the accumulation is never zeroed. Thus the output of correlation data at any timestep is the average over samples accumulated every Nevery steps since the fix was defined. it can only be restarted by deleting the fix via the unfix command, or by re-defining the fix by re-specifying it.

The start keyword specifies what timestep the accumulation of correlation samples will begin on. The default is step 0. Setting it to a larger value can avoid adding non-equilibrated data to the correlation averages.

The prefactor keyword specifies a constant which will be used as a multiplier on the correlation data after it is averaged. It is effectively a scale factor on Vi*Vj, which can be used to account for the size of the time window or other unit conversions.
The *file* keyword allows a filename to be specified. Every \( Nfreq \) steps, an array of correlation data is written to the file. The number of rows is \( Nrepeat \), as described above. The number of columns is the \( Npair+2 \), also as described above. Thus the file ends up to be a series of these array sections.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Time-correlated data for fix ID
# TimeStep Number-of-time-windows
# Index TimeDelta Ncount valueI*valueJ valueI*valueJ ...
```

In the first line, ID is replaced with the fix-ID. The second line describes the two values that are printed at the first of each section of output. In the third line the value pairs are replaced with the appropriate fields from the fix *ave/correlate* command.

Let \( S_{ij} \) = a set of time correlation data for input values I and J, namely the \( Nrepeat \) values:

\[
S_{ij} = C_{ij}(0), C_{ij}(N\text{every}), C_{ij}(2\times N\text{every}), \ldots, C_{ij}((N-1)\times N\text{every})
\]

As explained below, these datums are output as one column of a global array, which is effectively the correlation matrix.

The *trap* function defined for *equal-style* variables can be used to perform a time integration of this vector of datums, using a trapezoidal rule. This is useful for calculating various quantities which can be derived from time correlation data. If a normalization factor is needed for the time integration, it can be included in the variable formula or via the *prefactor* keyword.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the *fix_modify* options are relevant to this fix.

This fix computes a global array of values which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of \( Nfreq \) since that is when averaging is performed. The global array has \# of rows = \( Nrepeat \) and \# of columns = \( Npair+2 \). The first column has the time delta (in timesteps) between the pairs of input values used to calculate the correlation, as described above. The 2nd column has the number of samples contributing to the correlation average, as described above. The remaining \( Npair \) columns are for I,J pairs of the \( N \) input values, as determined by the *type* keyword, as described above.

- For *type* = *auto*, the \( Npair = N \) columns are ordered: \( C_{11}, C_{22}, \ldots, C_{NN} \).
- For *type* = *upper*, the \( Npair = N\times(N-1)/2 \) columns are ordered: \( C_{12}, C_{13}, \ldots, C_{1N}, C_{23}, \ldots, C_{2N}, C_{34}, \ldots, C_{N-1N} \).
- For *type* = *lower*, the \( Npair = N\times(N-1)/2 \) columns are ordered: \( C_{21}, C_{31}, C_{32}, C_{41}, C_{42}, C_{43}, \ldots, C_{N1}, C_{N2}, \ldots, C_{NN-1} \).
- For *type* = *auto/upper*, the \( Npair = N\times(N+1)/2 \) columns are ordered: \( C_{11}, C_{12}, C_{13}, \ldots, C_{1N}, C_{22}, C_{23}, \ldots, C_{2N}, C_{33}, C_{34}, \ldots, C_{N-1N}, C_{NN} \).
• For type = auto/\lower, the Npair = N*(N+1)/2 columns are ordered: C11, C21, C22, C31, C32, C33, C41, ..., C44, CN1, CN2, ..., CNN-1, CNN.

• For type = full, the Npair = N^2 columns are ordered: C11, C12, ..., C1N, C21, C22, ..., C2N, C31, ..., C3N, ..., CN1, ..., CNN-1, CNN.

The array values calculated by this fix are treated as "intensive". If you need to divide them by the number of atoms, you must do this in a later processing step, e.g. when using them in a variable.

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:
compute, fix ave/time, fix ave/atom, fix ave/spatial, fix ave/histo, variable

Default: none

The option defaults are ave = one, type = auto, start = 0, no file output, title 1,2,3 = strings as described above, and prefactor = 1.0.
fix ave/histo command

Syntax:

fix ID group-ID ave/histo Nevery Nrepeat Nfreq lo hi Nbin value1 value2 ... keyword args ...

- ID, group-ID are documented in fix command
- ave/histo = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating histogram
- Nfreq = calculate histogram every this many timesteps
- lo, hi = lo/hi bounds within which to histogram
- Nbin = # of histogram bins
- one or more input values can be listed
- value = x, y, z, vx, vy, vz, fx, fy, fz, c_ID, c_ID[N], f_ID, f_ID[N], v_name
  - x, y, z, vx, vy, vz, fx, fy, fz = atom attribute (position, velocity, force component)
  - c_ID = scalar or vector calculated by a compute with ID
  - c_ID[I] = Ith component of vector or Ith column of array calculated by a compute with ID
  - f_ID = scalar or vector calculated by a fix with ID
  - f_ID[I] = Ith component of vector or Ith column of array calculated by a fix with ID
  - v_name = value(s) calculated by an equal-style or atom-style variable with name
- zero or more keyword/arg pairs may be appended
- keyword = mode or file or ave or start or beyond or overwrite or title1 or title2 or title3

  mode arg = scalar or vector
  scalar = all input values are scalars
  vector = all input values are vectors
  file arg = filename
  filename = name of file to output histogram(s) to
  ave arg = one or running or window
  one = output a new average value every Nfreq steps
  running = output cumulative average of all previous Nfreq steps
  window M = output average of M most recent Nfreq steps
  start arg = Nstart
  Nstart = start averaging on this timestep
  beyond arg = ignore or end or extra
  ignore = ignore values outside histogram lo/hi bounds
  end = count values outside histogram lo/hi bounds in end bins
  extra = create 2 extra bins for value outside histogram lo/hi bounds
  overwrite arg = none = overwrite output file with only latest output
  title1 arg = string
  string = text to print as 1st line of output file
  title2 arg = string
  string = text to print as 2nd line of output file
  title3 arg = string
  string = text to print as 3rd line of output file, only for vector mode

Examples:

fix 1 all ave/histo 100 5 1000 0.5 1.5 50 c_myTemp file temp.histo ave running
fix 1 all ave/histo 100 5 1000 -5 5 100 c_thermo_press[2] c_thermo_press[3] title1 "My output values"
fix 1 all ave/histo 1 100 1000 -2.0 2.0 18 vx vy vz mode vector ave running beyond extra

Description:
Use one or more values as inputs every few timesteps, histogram them, and average the histogram over longer timescales. The resulting histogram can be used by other output commands, and can also be written to a file.

The group specified with this command is ignored for global and local input values. For per-atom input values, only atoms in the group contribute to the histogram. Note that regardless of the specified group, specified values may represent calculations performed by computes and fixes which store their own "group" definition.

A histogram is simply a count of the number of values that fall within a histogram bin. \textit{Nbins} are defined, with even spacing between \textit{lo} and \textit{hi}. Values that fall outside the \textit{lo}/\textit{hi} bounds can be treated in different ways; see the discussion of the \textit{beyond} keyword below.

Each input value can be an atom attribute (position, velocity, force component) or can be the result of a compute or fix or the evaluation of an equal-style or atom-style variable. The set of input values can be either all global, all per-atom, or all local quantities. Inputs of different kinds (e.g. global and per-atom) cannot be mixed. Atom attributes are per-atom vector values. See the doc page for individual "compute" and "fix" commands to see what kinds of quantities they generate.

The input values must either be all scalars or all vectors (or arrays), depending on the setting of the mode keyword.

If \textit{mode} = vector, then the input values may either be vectors or arrays. If a global array is listed, then it is the same as if the individual columns of the array had been listed one by one. E.g. these 2 fix ave/histo commands are equivalent, since the compute com/molecule command creates a global array with 3 columns:

\begin{verbatim}
compute myCOM all com/molecule
fix 1 all ave/histo 100 1 100 c_myCOM file tmpl.com mode vector
\end{verbatim}

The output of this command is a single histogram for all input values combined together, not one histogram per input value. See below for details on the format of the output of this fix.

The \textit{Nevery}, \textit{Nrepeat}, and \textit{Nfreq} arguments specify on what timesteps the input values will be used in order to contribute to the histogram. The final histogram is generated on timesteps that are multiple of \textit{Nfreq}. It is averaged over \textit{Nrepeat} histograms, computed in the preceding portion of the simulation every \textit{Nevery} timesteps. \textit{Nfreq} must be a multiple of \textit{Nevery} and \textit{Nevery} must be non-zero even if \textit{Nrepeat} is 1. Also, the timesteps contributing to the histogram cannot overlap, i.e. \textit{Nfreq} > (\textit{Nrepeat}-1)*\textit{Nevery} is required.

For example, if \textit{Nevery}=2, \textit{Nrepeat}=6, and \textit{Nfreq}=100, then input values on timesteps 90,92,94,96,98,100 will be used to compute the final histogram on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If \textit{Nrepeat}=1 and \textit{Nfreq} = 100, then no time averaging of the histogram is done; a histogram is simply generated on timesteps 100,200,etc.

The atom attribute values (x,y,z,vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes can be used as inputs to this fix by using the compute property/atom command and then specifying an input value from that compute.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If \textit{mode} = scalar, then if no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used. If \textit{mode} = vector, then if no bracketed term is appended, the global or per-atom or local vector calculated by the compute is used. Or if the compute calculates an array, all of the columns of the array are used as if they had been specified as individual vectors (see description above). If a bracketed term is appended, the Ith column of the global or per-atom or local array calculated by the compute is used.
Note that there is a compute reduce command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix ave/histo. Or it can be a compute defined not in your input script, but by thermodynamic output or other fixes such as fix nvt or fix temp/rescale. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If mode = scalar, then if no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used. If mode = vector, then if no bracketed term is appended, the global or per-atom or local vector calculated by the fix is used. Or if the fix calculates an array, all of the columns of the array are used as if they had been specified as individual vectors (see description above). If a bracketed term is appended, the Ith column of the global or per-atom or local array calculated by the fix is used.

Note that some fixes only produce their values on certain timesteps, which must be compatible with Nevery, else an error will result. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. If mode = scalar, then only equal-style variables can be used, which produce a global value. If mode = vector, then only atom-style variables can be used, which produce a per-atom vector. See the variable command for details. Note that variables of style equal and atom define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to histogram.

Additional optional keywords also affect the operation of this fix.

If the mode keyword is set to scalar, then all input values must be global scalars, or elements of global vectors. If the mode keyword is set to vector, then all input values must be global or per-atom or local vectors, or columns of global or per-atom or local arrays.

The beyond keyword determines how input values that fall outside the lo to hi bounds are treated. Values such that lo <= value <= hi are assigned to one bin. Values on a bin boundary are assigned to the lower of the 2 bins. If beyond is set to ignore then values < lo and values > hi are ignored, i.e. they are not binned. If beyond is set to end then values < lo are counted in the first bin and values > hi are counted in the last bin. If beyond is set to extend then two extra bins are created, so that there are Nbins+2 total bins. Values < lo are counted in the first bin and values > hi are counted in the last bin (Nbins+1). Values between lo and hi (inclusive) are counted in bins 2 thru Nbins+1. The "coordinate" stored and printed for these two extra bins is lo and hi.

The ave keyword determines how the histogram produced every Nfreq steps are averaged with histograms produced on previous steps that were multiples of Nfreq, before they are accessed by another output command or written to a file.

If the ave setting is one, then the histograms produced on timesteps that are multiples of Nfreq are independent of each other; they are output as-is without further averaging.

If the ave setting is running, then the histograms produced on timesteps that are multiples of Nfreq are summed and averaged in a cumulative sense before being output. Each bin value in the histogram is thus the average of the bin value produced on that timestep with all preceding values for the same bin. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the unfix command, or by re-defining the fix by re-specifying it.
If the ave setting is window, then the histograms produced on timesteps that are multiples of $Nfreq$ are summed within a moving "window" of time, so that the last $M$ histograms are used to produce the output. E.g. if $M = 3$ and $Nfreq = 1000$, then the output on step 10000 will be the combined histogram of the individual histograms on steps 8000, 9000, 10000. Outputs on early steps will be sums over less than $M$ histograms if they are not available.

The start keyword specifies what timestep histogramming will begin on. The default is step 0. Often input values can be 0.0 at time 0, so setting start to a larger value can avoid including a 0.0 in a running or windowed histogram.

The file keyword allows a filename to be specified. Every $Nfreq$ steps, one histogram is written to the file. This includes a leading line that contains the timestep, number of bins, the total count of values contributing to the histogram, the count of values that were not histogrammed (see the beyond keyword), the minimum value encountered, and the maximum value encountered. The min/max values include values that were not histogrammed. Following the leading line, one line per bin is written into the file. Each line contains the bin #, the coordinate for the center of the bin (between $lo$ and $hi$), the count of values in the bin, and the normalized count. The normalized count is the bin count divided by the total count (not including values not histogrammed), so that the normalized values sum to 1.0 across all bins.

The overwrite keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the ave running setting.

The title1 and title2 and title3 keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the file keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Histogram for fix ID
# TimeStep Number-of-bins Total-counts Missing-counts Min-value Max-value
# Bin Coord Count Count/Total
```

In the first line, ID is replaced with the fix-ID. The second line describes the six values that are printed at the first of each section of output. The third describes the 4 values printed for each bin in the histogram.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix produces a global vector and global array which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of $Nfreq$ since that is when a histogram is generated. The global vector has 4 values:

- $1 =$ total counts in the histogram
- $2 =$ values that were not histogrammed (see beyond keyword)
- $3 =$ min value of all input values, including ones not histogrammed
- $4 =$ max value of all input values, including ones not histogrammed

The global array has # of rows = Nbins and # of columns = 3. The first column has the bin coordinate, the 2nd column has the count of values in that histogram bin, and the 3rd column has the bin count divided by the total count (not including missing counts), so that the values in the 3rd column sum to 1.0.
The vector and array values calculated by this fix are all treated as "intensive". If this is not the case, e.g. due to histogramming per-atom input values, then you will need to account for that when interpreting the values produced by this fix.

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

compute, fix ave/atom, fix ave/spatial, fix ave/time, variable, fix ave/correlate,

**Default:** none

The option defaults are mode = scalar, ave = one, start = 0, no file output, beyond = ignore, and title 1,2,3 = strings as described above.
fix ave/spatial command

Syntax:

fix ID group-ID ave/spatial Nevery Nrepeat Nfreq dim origin delta ... value1 value2 ... keyword args ...

• ID, group-ID are documented in fix command
• ave/spatial = style name of this fix command
• Nevery = use input values every this many timesteps
• Nrepeat = # of times to use input values for calculating averages
• Nfreq = calculate averages every this many timesteps
• dim, origin, delta can be repeated 1, 2, or 3 times for 1d, 2d, or 3d bins

    dim = x or y or z
    origin = lower or center or upper or coordinate value (distance units)
    delta = thickness of spatial bins in dim (distance units)

• one or more input values can be listed
• value = vx, vy, vz, fx, fy, fz, density/mass, density/number, c_ID, c_ID[I], f_ID, f_ID[I], v_name

    vx,vy,vz,fx,fy,fz = atom attribute (velocity, force component)
    density/number, density/mass = number or mass density
    c_ID = per-atom vector calculated by a compute with ID
    c_ID[I] = Ith column of per-atom array calculated by a compute with ID
    f_ID = per-atom vector calculated by a fix with ID
    f_ID[I] = Ith column of per-atom array calculated by a fix with ID
    v_name = per-atom vector calculated by an atom-style variable with name

• zero or more keyword/arg pairs may be appended
• keyword = norm or units or file or ave or overwrite or title1 or title2 or title3

    units arg = box or lattice or reduced
    norm arg = all or sample
    region arg = region-ID
    region-ID = ID of region atoms must be in to contribute to spatial averaging
    ave arg = one or running or window M
    one = output new average value every Nfreq steps
    running = output cumulative average of all previous Nfreq steps
    window M = output average of M most recent Nfreq steps
    file arg = filename
    filename = file to write results to
    overwrite arg = none = overwrite output file with only latest output
    title1 arg = string
    string = text to print as 1st line of output file
    title2 arg = string
    string = text to print as 2nd line of output file
    title3 arg = string
    string = text to print as 3rd line of output file

Examples:

fix 1 all ave/spatial 10000 1 10000 z lower 0.02 c_myCentro units reduced &
    title1 "My output values"
fix 1 flow ave/spatial 100 10 1000 y 0.0 1.0 vx vz norm sample file vel.profile
fix 1 flow ave/spatial 100 5 1000 z lower 1.0 y 0.0 2.5 density/mass ave running

Description:
Use one or more per-atom vectors as inputs every few timesteps, bin their values spatially into 1d, 2d, or 3d bins based on current atom coordinates, and average the bin values over longer timescales. The resulting bin averages can be used by other output commands such as thermo_style custom, and can also be written to a file.

The group specified with the command means only atoms within the group contribute to bin averages. If the region keyword is used, the atom must be in both the group and the specified geometric region in order to contribute to bin averages.

Each listed value can be an atom attribute (position, velocity, force component), a mass or number density, or the result of a compute or fix or the evaluation of an atom-style variable. In the latter cases, the compute, fix, or variable must produce a per-atom quantity, not a global quantity. If you wish to time-average global quantities from a compute, fix, or variable, then see the fix ave/time command.

Computes that produce per-atom quantities are those which have the word atom in their style name. See the doc pages for individual fixes to determine which ones produce per-atom quantities. Variables of style atom are the only ones that can be used with this fix since all other styles of variable produce global quantities.

The per-atom values of each input vector are binned and averaged independently of the per-atom values in other input vectors.

The size and dimensionality of the bins (1d = layers or slabs, 2d = pencils, 3d = boxes) are determined by the dim, origin, and delta settings and how many times they are specified (1, 2, or 3). See details below.

IMPORTANT NOTE: This fix works by creating an array of size Nbins by Nvalues on each processor. Nbins is the total number of bins; Nvalues is the number of input values specified. Each processor loops over its atoms, tallying its values to the appropriate bin. Then the entire array is summed across all processors. This means that using a large number of bins (easy to do for 2d or 3d bins) will incur an overhead in memory and computational cost (summing across processors), so be careful to use reasonable numbers of bins.

The Nevery, Nrepeat, and Nfreq arguments specify on what timesteps the input values will be used to bin them and contribute to the average. The final averaged quantities are generated on timesteps that are a multiples of Nfreq. The average is over Nrepeat quantities, computed in the preceding portion of the simulation every Nevery timesteps. Nfreq must be a multiple of Nevery and Nevery must be non-zero even if Nrepeat is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nfreq > (Nrepeat-1)*Nevery is required.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

Each per-atom property is also averaged over atoms in each bin. Bins can be 1d layers or slabs, 2d pencils, or 3d boxes. This depends on how many times (1, 2, or 3) the dim, origin, and delta settings are specified in the fix ave/spatial command. For 2d or 3d bins, there is no restriction on specifying dim = x before dim = y, or dim = y before dim = z. Bins in a particular dim have a bin size in that dimension given by delta. Every Nfreq steps, when averaging is being performed and the per-atom property is calculated for the first time, the number of bins and the bin sizes and boundaries are computed. Thus if the simulation box changes size during a simulation, the number of bins and their boundaries may also change. In each dimension, bins are defined relative to a specified origin, which may be the lower/upper edge of the simulation box (in dim) or its center point, or a specified coordinate value. Starting at the origin, sufficient bins are created in both directions to completely cover the box. On subsequent timesteps every atom is mapped to one of the bins. Atoms beyond the lowermost/uppermost bin in a dimension are counted in the first/last bin in that dimension.
For orthogonal simulation boxes, the bins are also layers, pencils, or boxes aligned with the xyz coordinate axes. For triclinic (non-orthogonal) simulation boxes, the bins are so that they are parallel to the tilted faces of the simulation box. See this section of the manual for a discussion of the geometry of triclinic boxes in LAMMPS. As described there, a tilted simulation box has edge vectors a,b,c. In that nomenclature, bins in the x dimension have faces with normals in the "b" cross "c" direction. Bins in y have faces normal to the "a" cross "c" direction. And bins in z have faces normal to the "a" cross "b" direction. Note that in order to define the size and position of these bins in an unambiguous fashion, the units option must be set to reduced when using a triclinic simulation box, as noted below.

The atom attribute values (vx,vy,vz,fx, fy, fz) are self-explanatory. Note that other atom attributes (including atom positions x, y, z) can be used as inputs to this fix by using the compute property/atom command and then specifying an input value from that compute.

The density/number value means the number density is computed in each bin, i.e. a weighting of 1 for each atom. The density/mass value means the mass density is computed in each bin, i.e. each atom is weighted by its mass. The resulting density is normalized by the volume of the bin so that units of number/volume or density are output. See the units command doc page for the definition of density for each choice of units, e.g. gram/cm^3.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with Nevery, else an error results. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Variables of style atom can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to spatially average.

Additional optional keywords also affect the operation of this fix.

The units keyword determines the meaning of the distance units used for the bin size delta and for origin if it is a coordinate value. For orthogonal simulation boxes, any of the 3 options may be used. For non-orthogonal (triclinic) simulation boxes, only the reduced option may be used.

A box value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A lattice value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. A reduced value means normalized unitless values between 0 and 1, which represent the lower and upper faces of the simulation box respectively. Thus an origin value of 0.5 means the center of the box in any dimension. A delta value of 0.1 means 10 bins span the box in that dimension.

Consider a non-orthogonal box, with bins that are 1d layers or slabs in the x dimension. No matter how the box is tilted, an origin of 0.0 means start layers at the lower "b" cross "c" plane of the simulation box and an origin of 1.0 means to start layers at the upper "b" cross "c" face of the box. A delta value of 0.1 means there will be 10 layers from 0.0 to 1.0, regardless of the current size or shape of the simulation box.
The `norm` keyword affects how averaging is done for the output produced every `Nfreq` timesteps. For an `all` setting, a bin quantity is summed over all atoms in all `Nrepeat` samples, as is the count of atoms in the bin. The printed value for the bin is `Total-quantity / Total-count`. In other words it is an average over the entire `Nfreq` timescale.

For a `sample` setting, the bin quantity is summed over atoms for only a single sample, as is the count, and a "average sample value" is computed, i.e. `Sample-quantity / Sample-count`. The printed value for the bin is the average of the `Nrepeat" average sample values", In other words it is an average of an average.

The `ave` keyword determines how the bin values produced every `Nfreq` steps are averaged with bin values produced on previous steps that were multiples of `Nfreq`, before they are accessed by another output command or written to a file.

If the `ave` setting is `one`, then the bin values produced on timesteps that are multiples of `Nfreq` are independent of each other; they are output as-is without further averaging.

If the `ave` setting is `running`, then the bin values produced on timesteps that are multiples of `Nfreq` are summed and averaged in a cumulative sense before being output. Each output bin value is thus the average of the bin value produced on that timestep with all preceding values for the same bin. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the `unfix` command, or re-defining the fix by re-specifying it.

If the `ave` setting is `window`, then the bin values produced on timesteps that are multiples of `Nfreq` are summed and averaged within a moving "window" of time, so that the last `M` values for the same bin are used to produce the output. E.g. if `M = 3` and `Nfreq = 1000`, then the output on step 10000 will be the average of the individual bin values on steps 8000,9000,10000. Outputs on early steps will average over less than `M` values if they are not available.

The `file` keyword allows a filename to be specified. Every `Nfreq` timesteps, a section of bin info will be written to a text file in the following format. A line with the timestep and number of bin is written. Then one line per bin is written, containing the bin ID (1-N), the coordinate of the center of the bin, the number of atoms in the bin, and one or more calculated values. The number of values in each line corresponds to the number of values specified in the fix `ave/spatial` command. The number of atoms and the value(s) are average quantities. If the value of the `units` keyword is `box` or `lattice`, the "coord" is printed in box units. If the value of the `units` keyword is `reduced`, the "coord" is printed in reduced units (0-1).

The `overwrite` keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the `ave running` setting.

The `title1` and `title2` and `title3` keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the `file` keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Spatial-averaged data for fix ID and group name
# Timestep Number-of-bins
# Bin Coord1 Coord2 Coord3 Count value1 value2 ...
```

In the first line, ID and name are replaced with the fix-ID and group name. The second line describes the two values that are printed at the first of each section of output. In the third line the values are replaced with the appropriate fields from the fix `ave/spatial` command. The Coord2 and Coord3 entries in the third line only appear for 2d and 3d bins respectively. For 1d bins, the word Coord1 is replaced by just Coord.
Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global array of values which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of Nfreq since that is when averaging is performed. The global array has # of rows = Nbins and # of columns = Ndim+1+Nvalues, where Ndim = 1,2,3 for 1d,2d,3d bins. The first 1 or 2 or 3 columns have the bin coordinates (center of the bin) in the appropriate dimensions, the next column has the count of atoms in that bin, and the remaining columns are the Nvalue quantities. When the array is accessed with an I that exceeds the current number of bins, than a 0.0 is returned by the fix instead of an error, since the number of bins can vary as a simulation runs, depending on the simulation box size. 2d or 3d bins are ordered so that the last dimension(s) vary fastest. The array values calculated by this fix are "intensive", since they are already normalized by the count of atoms in each bin.

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

When the ave keyword is set to running or window then the number of bins must remain the same during the simulation, so that the appropriate averaging can be done. This will be the case if the simulation box size doesn't change or if the units keyword is set to reduced.

Related commands:

compute, fix ave/atom, fix ave/histo, fix ave/time, variable, fix ave/correlate,

Default:

The option defaults are units = lattice, norm = all, no file output, and ave = one, title 1,2,3 = strings as described above.
**fix ave/time command**

Syntax:

```plaintext
fix ID group-ID ave/time Nevery Nrepeat Nfreq value1 value2 ... keyword args ...
```

- ID, group-ID are documented in `fix` command
- `ave/time` = style name of this fix command
- `Nevery` = use input values every this many timesteps
- `Nrepeat` = # of times to use input values for calculating averages
- `Nfreq` = calculate averages every this many timesteps
- one or more input values can be listed
- `value = c_ID, c_ID[N], f_ID, f_ID[N], v_name`
  - `c_ID` = global scalar or vector calculated by a compute with ID
  - `c_ID[N]` = Ith component of global vector or Ith column of global array calculated by a compute with ID
  - `f_ID` = global scalar or vector calculated by a fix with ID
  - `f_ID[N]` = Ith component of global vector or Ith column of global array calculated by a fix with ID
  - `v_name` = global value calculated by an equal-style variable with name
- zero or more keyword/arg pairs may be appended
- `keyword = mode` or `file` or `ave` or `start` or `off` or `overwrite` or `title1` or `title2` or `title3`

  - `mode arg = scalar` or `vector`
    - `scalar` = all input values are global scalars
    - `vector` = all input values are global vectors or global arrays
  - `ave arg = one` or `running` or `window M`
    - `one` = output a new average value every Nfreq steps
    - `running` = output cumulative average of all previous Nfreq steps
    - `window M` = output average of M most recent Nfreq steps
  - `start args = Nstart`
    - `Nstart` = start averaging on this timestep
  - `off arg = M = do not average this value`
    - `M` = value # from 1 to Nvalues
  - `file arg = filename`
    - `filename` = name of file to output time averages to
  - `overwrite arg = none = overwrite output file with only latest output`
  - `title1 arg = string`
    - `string` = text to print as 1st line of output file
  - `title2 arg = string`
    - `string` = text to print as 2nd line of output file
  - `title3 arg = string`
    - `string` = text to print as 3rd line of output file, only for vector mode

**Examples:**

```plaintext
fix 1 all ave/time 100 5 1000 c_myTemp c_thermo_temp file temp.profile
fix 1 all ave/time 100 5 1000 c_thermo_press[2] ave window 20 &
  title1 "My output values"
fix 1 all ave/time 1 100 1000 f_indent f_indent[1] file temp.indent off 1
```

**Description:**

Use one or more global values as inputs every few timesteps, and average them over longer timescales. The resulting averages can be used by other output commands such as `thermo_style custom`, and can also be written to a file. Note that if no time averaging is done, this command can be used as a convenient way to simply output one
or more global values to a file.

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a compute or fix or the evaluation of an equal-style variable. In each case, the compute, fix, or variable must produce a global quantity, not a per-atom or local quantity. If you wish to spatial- or time-average or histogram per-atom quantities from a compute, fix, or variable, then see the fix ave/spatial, fix ave/atom, or fix ave/histo commands. If you wish to sum a per-atom quantity into a single global quantity, see the compute reduce command.

Computes that produce global quantities are those which do not have the word atom in their style name. Only a few fixes produce global quantities. See the doc pages for individual fixes for info on which ones produce such values. Variables of style equal are the only ones that can be used with this fix. Variables of style atom cannot be used, since they produce per-atom values.

The input values must either be all scalars or all vectors (or arrays), depending on the setting of the mode keyword. In both cases, the averaging is performed independently on each input value. I.e. each input scalar is averaged independently and each element of each input vector (or array) is averaged independently.

If mode = vector, then the input values may either be vectors or arrays and all must be the same "length", which is the length of the vector or number of rows in the array. If a global array is listed, then it is the same as if the individual columns of the array had been listed one by one. E.g. these 2 fix ave/time commands are equivalent, since the compute rdf command creates, in this case, a global array with 3 columns, each of length 50:

```
compute myRDF all rdf 50 1 2
fix 1 all ave/time 100 1 100 c_myRDF file tmp1.rdf mode vector
```

The Nevery, Nrepeat, and Nfreq arguments specify on what timesteps the input values will be used in order to contribute to the average. The final averaged quantities are generated on timesteps that are a multiple of Nfreq. The average is over Nrepeat quantities, computed in the preceding portion of the simulation every Nevery timesteps. Nfreq must be a multiple of Nevery and Nevery must be non-zero even if Nrepeat is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nfreq > (Nrepeat-1)*Nevery is required.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If mode = scalar, then if no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used. If mode = vector, then if no bracketed term is appended, the global vector calculated by the compute is used. Or if the compute calculates an array, all of the columns of the global array are used as if they had been specified as individual vectors (see description above). If a bracketed term is appended, the Ith column of the global array calculated by the compute is used.

Note that there is a compute reduce command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix ave/time. Or it can be a compute defined not in your input script, but by thermodynamic output or other fixes such as fix nvt or fix temp/rescale. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and add them to LAMMPS.
If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If \textit{mode} = scalar, then if no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the \textit{Ith} element of the global vector calculated by the fix is used. If \textit{mode} = vector, then if no bracketed term is appended, the global vector calculated by the fix is used. Or if the fix calculates an array, all of the columns of the global array are used as if they had been specified as individual vectors (see description above). If a bracketed term is appended, the \textit{Ith} column of the global array calculated by the fix is used.

Note that some fixes only produce their values on certain timesteps, which must be compatible with \textit{Nevery}, else an error will result. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Variables can only be used as input for \textit{mode} = scalar. Only equal-style variables can be referenced. See the \texttt{variable} command for details. Note that variables of style \textit{equal} define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to time average.

Additional optional keywords also affect the operation of this fix.

If the \textit{mode} keyword is set to \textit{scalar}, then all input values must be global scalars, or elements of global vectors. If the \textit{mode} keyword is set to \textit{vector}, then all input values must be global vectors, or columns of global arrays. They can also be global arrays, which are converted into a series of global vectors (one per column), as explained above.

The \textit{ave} keyword determines how the values produced every \textit{Nfreq} steps are averaged with values produced on previous steps that were multiples of \textit{Nfreq}, before they are accessed by another output command or written to a file.

If the \textit{ave} setting is \textit{one}, then the values produced on timesteps that are multiples of \textit{Nfreq} are independent of each other; they are output as-is without further averaging.

If the \textit{ave} setting is \textit{running}, then the values produced on timesteps that are multiples of \textit{Nfreq} are summed and averaged in a cumulative sense before being output. Each output value is thus the average of the value produced on that timestep with all preceding values. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the \texttt{unfix} command, or by re-defining the fix by re-specifying it.

If the \textit{ave} setting is \textit{window}, then the values produced on timesteps that are multiples of \textit{Nfreq} are summed and averaged within a moving "window" of time, so that the last \textit{M} values are used to produce the output. E.g. if \textit{M} = 3 and \textit{Nfreq} = 1000, then the output on step 10000 will be the average of the individual values on steps 8000,9000,10000. Outputs on early steps will average over less than \textit{M} values if they are not available.

The \textit{start} keyword specifies what timestep averaging will begin on. The default is step 0. Often input values can be 0.0 at time 0, so setting \textit{start} to a larger value can avoid including a 0.0 in a running or windowed average.

The \textit{off} keyword can be used to flag any of the input values. If a value is flagged, it will not be time averaged. Instead the most recent input value will always be stored and output. This is useful if one of more of the inputs produced by a compute or fix or variable are effectively constant or are simply current values. E.g. they are being written to a file with other time-averaged values for purposes of creating well-formatted output.

The \textit{file} keyword allows a filename to be specified. Every \textit{Nfreq} steps, one quantity or vector of quantities is written to the file for each input value specified in the fix \textit{ave/time} command. For \textit{mode} = scalar, this means a single line is written each time output is performed. Thus the file ends up to be a series of lines, i.e. one column of numbers for each input value. For \textit{mode} = vector, an array of numbers is written each time output is performed.
The number of rows is the length of the input vectors, and the number of columns is the number of values. Thus the file ends up to be a series of these array sections.

The `overwrite` keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the `ave running` setting.

The `title1` and `title2` and `title3` keywords allow specification of the strings that will be printed as the first 2 or 3 lines of the output file, assuming the `file` keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows for `mode = scalar`:

```
# Time-averaged data for fix ID
# TimeStep value1 value2 ...
```

In the first line, ID is replaced with the fix-ID. In the second line the values are replaced with the appropriate fields from the fix `ave/time` command. There is no third line in the header of the file, so the `title3` setting is ignored when `mode = scalar`.

By default, these header lines are as follows for `mode = vector`:

```
# Time-averaged data for fix ID
# TimeStep Number-of-rows
# Row value1 value2 ...
```

In the first line, ID is replaced with the fix-ID. The second line describes the two values that are printed at the first of each section of output. In the third line the values are replaced with the appropriate fields from the fix `ave/time` command.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the `fix_modify` options are relevant to this fix.

This fix produces a global scalar or global vector or global array which can be accessed by various `output commands`. The values can only be accessed on timesteps that are multiples of `Nfreq` since that is when averaging is performed.

A scalar is produced if only a single input value is averaged and `mode = scalar`. A vector is produced if multiple input values are averaged for `mode = scalar`, or a single input value for `mode = vector`. In the first case, the length of the vector is the number of inputs. In the second case, the length of the vector is the same as the length of the input vector. An array is produced if multiple input values are averaged and `mode = vector`. The global array has # of rows = length of the input vectors and # of columns = number of inputs.

If the fix produces a scalar or vector, then the scalar and each element of the vector can be either "intensive" or "extensive". If the fix produces an array, then all elements in the array must be the same, either "intensive" or "extensive". If a compute or fix provides the value being time averaged, then the compute or fix determines whether the value is intensive or extensive; see the doc page for that compute or fix for further info. Values produced by a variable are treated as intensive.

No parameter of this fix can be used with the `start/stop` keywords of the `run` command. This fix is not invoked during `energy minimization`.
Restrictions: none

Related commands:

compute, fix ave/atom, fix ave/spatial, fix ave/histo, variable, fix ave/correlate,

Default: none

The option defaults are mode = scalar, ave = one, start = 0, no file output, title 1,2,3 = strings as described above, and no off settings for any input values.
fix aveforce command

fix aveforce/cuda command

Syntax:

fix ID group-ID aveforce fx fy fz keyword value ...

• ID, group-ID are documented in fix command
• aveforce = style name of this fix command
• fx, fy, fz = force component values (force units)

  any of fx, fy, fz can be a variable (see below)
• zero or more keyword/value pairs may be appended to args
• keyword = region

  region value = region-ID
  region-ID = ID of region atoms must be in to have added force

Examples:

fix pressdown topwall aveforce 0.0 -1.0 0.0
fix 2 bottomwall aveforce NULL -1.0 0.0 region top
fix 2 bottomwall aveforce NULL -1.0 v_oscillate region top

Description:

Apply an additional external force to a group of atoms in such a way that every atom experiences the same force. This is useful for pushing on wall or boundary atoms so that the structure of the wall does not change over time.

The existing force is averaged for the group of atoms, component by component. The actual force on each atom is then set to the average value plus the component specified in this command. This means each atom in the group receives the same force.

Any of the fx, fy, fz values can be specified as NULL which means the force in that dimension is not changed. Note that this is not the same as specifying a 0.0 value, since that sets all forces to the same average value without adding in any additional force.

Any of the 3 quantities defining the force components can be specified as an equal-style variable, namely fx, fy, fz. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the average force.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent average force.

If the region keyword is used, the atom must also be in the specified geometric region in order to have force added to it.

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual.
The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various output commands. This is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. You should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

**Restrictions:** none

**Related commands:**

fix setforce, fix addforce

**Default:** none
fix balance command

Syntax:

fix ID group-ID balance Nfreq dimstr Niter thresh keyword value ...

- ID, group-ID are documented in fix command
- balance = style name of this fix command
- Nfreq = perform dynamic load balancing every this many steps
- dimstr = sequence of letters containing "x" or "y" or "z", each not more than once
- Niter = # of times to iterate within each dimension of dimstr sequence
- thresh = stop balancing when this imbalance threshold is reached
- zero or more keyword/arg pairs may be appended

- keyword = out

    out arg = filename
    filename = output file to write each processor's sub-domain to

Examples:

fix 2 all balance 1000 x 10 1.05
fix 2 all balance 0 xy 20 1.1 out tmp.balance

Description:

This command adjusts the size of processor sub-domains within the simulation box dynamically as a simulation runs, to attempt to balance the number of particles and thus the computational cost (load) evenly across processors. The load balancing is "dynamic" in the sense that rebalancing is performed periodically during the simulation. To perform "static" balancing, before or between runs, see the balance command.

Load-balancing is only useful if the particles in the simulation box have a spatially-varying density distribution. E.g. a model of a vapor/liquid interface, or a solid with an irregular-shaped geometry containing void regions. In this case, the LAMMPS default of dividing the simulation box volume into a regular-spaced grid of processor sub-domain, with one equal-volume sub-domain per processor, may assign very different numbers of particles per processor. This can lead to poor performance in a scalability sense, when the simulation is run in parallel.

Note that the processors command gives you some control over how the box volume is split across processors. Specifically, for a Px by Py by Pz grid of processors, it lets you choose Px, Py, and Pz, subject to the constraint that Px * Py * Pz = P, the total number of processors. This can be sufficient to achieve good load-balance for some models on some processor counts. However, all the processor sub-domains will still be the same shape and have the same volume.

This command does not alter the topology of the Px by Py by Pz grid or processors. But it shifts the cutting planes between processors (in 3d, or lines in 2d), which adjusts the volume (area in 2d) assigned to each processor, as in the following 2d diagram. The left diagram is the default partitioning of the simulation box across processors (one sub-box for each of 16 processors); the right diagram is after balancing.
IMPORTANT NOTE: This command attempts to minimize the imbalance factor, as defined above. But because of the topology constraint that only the cutting planes (lines) between processors are moved, there are many irregular distributions of particles, where this factor cannot be shrunk to 1.0, particularly in 3d. Also, computational cost is not strictly proportional to particle count, and changing the relative size and shape of processor sub-domains may lead to additional computational and communication overheads, e.g. in the PPPM solver used via the kspace_style command. Thus you should benchmark the run times of your simulation with and without balancing.

The group-ID is currently ignored. In the future it may be used to determine what particles are considered for balancing. Normally it would only makes sense to use the all group. But in some cases it may be useful to balance on a subset of the particles, e.g. when modeling large nanoparticles in a background of small solvent particles.

The Nfreq setting determines how often a rebalance is performed. If Nfreq > 0, then rebalancing will occur every Nfreq steps. Each time a rebalance occurs, a reneighboring is triggered, so you should not make Nfreq too small. If Nfreq = 0, then rebalancing will be done every time reneighboring normally occurs, as determined by the the neighbor and neigh_modify command settings.

On rebalance steps, rebalancing will only be attempted if the current imbalance factor, as defined above, exceeds the thresh setting.

The dimstr argument is a string of characters, each of which must be an "x" or "y" or "z". Each character can appear zero or one time, since there is no advantage to balancing on a dimension more than once. You should normally only list dimensions where you expect there to be a density variation in the particles.

Balancing proceeds by adjusting the cutting planes in each of the dimensions listed in dimstr, one dimension at a time. For a single dimension, the balancing operation (described below) is iterated on up to Niter times. After each dimension finishes, the imbalance factor is re-computed, and the balancing operation halts if the thresh criterion is met.

A rebalance operation in a single dimension is performed using a density-dependent recursive multisectioning algorithm, where the position of each cutting plane (line in 2d) in the dimension is adjusted independently. This is similar to a recursive bisectioning (RCB) for a single value, except that the bounds used for each bisectioning take advantage of information from neighboring cuts if possible, as well as counts of particles at the bounds on either side of each cuts, which themselves were cuts in previous iterations. The latter is used to infer a density of particles near each of the current cuts. At each iteration, the count of particles on either side of each plane is tallied. If the counts do not match the target value for the plane, the position of the cut is adjusted based on the local density. The low and high bounds are adjusted on each iteration, using new count information, so that...
they become closer together over time. Thus as the recursion progresses, the count of particles on either side of the plane gets closer to the target value.

The density-dependent part of this algorithm is often an advantage when you rebalance a system that is already nearly balanced. It typically converges more quickly than the geometric bisectioning algorithm used by the balance command. However, if can be a disadvantage if you attempt to rebalance a system that is far from balanced, and converge more slowly. In this case you probably want to use the balance command before starting a run, so that you begin the run with a balanced system.

Once the rebalancing is complete and final processor sub-domains assigned, particles migrate to their new owning processor as part of the normal reneighboring procedure.

IMPORTANT NOTE: At each rebalance operation, the RCB operation for each cutting plane (line in 2d) typically starts with low and high bounds separated by the extent of a processor's sub-domain in one dimension. The size of this bracketing region shrinks based on the local density, as described above, which should typically be 1/2 or more every iteration. Thus if Niter is specified as 10, the cutting plane will typically be positioned to better than 1 part in 1000 accuracy (relative to the perfect target position). For Niter = 20, it will be accurate to better than 1 part in a million. Thus there is no need to set Niter to a large value. This is especially true if you are rebalancing often enough that each time you expect only an incremental adjustment in the cutting planes is necessary. LAMMPS will check if the threshold accuracy is reached (in a dimension) is less iterations than Niter and exit early.

IMPORTANT NOTE: If a portion of your system is a perfect lattice, e.g. a frozen substrate, then the balancer may be unable to achieve exact balance. I.e. entire lattice planes will be owned or not owned by a single processor. So you should not expect to achieve perfect balance in this case. Nor will it be helpful to use a large value for Niter, since it will simply cause the balancer to iterate until Niter is reached, without improving the imbalance factor.

The out keyword writes a text file to the specified filename with the results of each rebalancing operation. The file contains the bounds of the sub-domain for each processor after the balancing operation completes. The format of the file is compatible with the Pizza.py mdump tool which has support for manipulating and visualizing mesh files. An example is shown here for a balancing by 4 processors for a 2d problem:

```
ITEM: TIMESTEP
1000
ITEM: NUMBER OF SQUARES
4
ITEM: SQUARES
 1 1 1 2 7 6
 2 2 3 8 7
 3 3 4 9 8
 4 4 5 10 9
ITEM: TIMESTEP
1000
ITEM: NUMBER OF NODES
10
ITEM: BOX BOUNDS
-153.919 184.703
 0 15.3919
-0.769595 0.769595
ITEM: NODES
 1 1 -153.919 0 0
 2 1 7.45545 0 0
 3 1 14.7305 0 0
 4 1 22.667 0 0
 5 1 184.703 0 0
 6 1 -153.919 15.3919 0
```
The "SQUARES" lists the node IDs of the 4 vertices in a rectangle for each processor (1 to 4). The first SQUARE 1 (for processor 0) is a rectangle of type 1 (equal to SQUARE ID) and contains vertices 1,2,7,6. The coordinates of all the vertices are listed in the NODES section. Note that the 4 sub-domains share vertices, so there are only 10 unique vertices in total.

For a 3d problem, the syntax is similar with "SQUARES" replaced by "CUBES", and 8 vertices listed for each processor, instead of 4.

Each time rebalancing is performed a new timestamp is written with new NODES values. The SQUARES of CUBES sections are not repeated, since they do not change.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which is the imbalance factor after the most recent rebalance and a global vector of length 3 with additional information about the most recent rebalancing. The 3 values in the vector are as follows:

- 1 = max # of particles per processor
- 2 = total # iterations performed in last rebalance
- 3 = imbalance factor right before the last rebalance was performed

As explained above, the imbalance factor is the ratio of the maximum number of particles on any processor to the average number of particles per processor.

These quantities can be accessed by various output commands. The scalar and vector values calculated by this fix are "intensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

The fix balance command cannot yet be used with the long-range Coulombic PPPM solver invoked by kspace_style pppm.

**Related commands:**

processors, balance

**Default:** none
**fix bond/break command**

**Syntax:**

```
fix ID group-ID bond/break Nevery bondtype Rmax keyword values ...
```

- ID, group-ID are documented in `fix` command
- bond/break = style name of this fix command
- Nevery = attempt bond breaking every this many steps
- bondtype = type of bonds to break
- Rmax = bond longer than Rmax can break (distance units)
- zero or more keyword/value pairs may be appended to args
- keyword = `prob`

```
prob values = fraction seed
fraction = break a bond with this probability if otherwise eligible
seed = random number seed (positive integer)
```

**Examples:**

```
fix 5 all bond/break 10 2 1.2
fix 5 polymer bond/break 1 1 2.0 prob 0.5 49829
```

**Description:**

Break bonds between pairs of atoms as a simulation runs according to specified criteria. This can be used to model the dissolution of a polymer network due to stretching of the simulation box or other deformations. In this context, a bond means an interaction between a pair of atoms computed by the `bond_style` command. Once the bond is broken it will be permanently deleted. This is different than a pairwise bond-order potential such as Tersoff or AIREBO which infers bonds and many-body interactions based on the current geometry of a small cluster of atoms and effectively creates and destroys bonds from timestep to timestep as atoms move.

A check for possible bond breakage is performed every `Nevery` timesteps. If two bonded atoms I,J are further than a distance `Rmax` of each other, if the bond is of type `bondtype`, and if both I and J are in the specified fix group, then I,J is labeled as a "possible" bond to break. If several bonds involving an atom are stretched, it may have multiple possible bonds to break. Every atom checks its list of possible bonds to break and labels the longest such bond as its "sole" bond to break. After this is done, if atom I is bonded to atom J in its sole bond, and atom J is bonded to atom I in its sole bond, then the I,J bond is "eligible" to be broken.

Note that these rules mean an atom will only be part of at most one broken bond on a given timestep. It also means that if atom I chooses atom J as its sole partner, but atom J chooses atom K is its sole partner (due to Rjk > Rij), then this means atom I will not be part of a broken bond on this timestep, even if it has other possible bond partners.

The `prob` keyword can effect whether an eligible bond is actually broken. The `fraction` setting must be a value between 0.0 and 1.0. A uniform random number between 0.0 and 1.0 is generated and the eligible bond is only broken if the random number < fraction.
When a bond is broken, data structures within LAMMPS that store bond topology are updated to reflect the breakage. This can also affect subsequent computation of pairwise interactions involving the atoms in the bond. See the Restriction section below for additional information.

Computationally, each timestep this fix operates, it loops over bond lists and computes distances between pairs of bonded atoms in the list. It also communicates between neighboring processors to coordinate which bonds are broken. Thus it will increase the cost of a timestep. Thus you should be cautious about invoking this fix too frequently.

You can dump out snapshots of the current bond topology via the dump local command.

IMPORTANT NOTE: Breaking a bond typically alters the energy of a system. You should be careful not to choose bond breaking criteria that induce a dramatic change in energy. For example, if you define a very stiff harmonic bond and break it when 2 atoms are separated by a distance far from the equilibrium bond length, then the 2 atoms will be dramatically released when the bond is broken. More generally, you may need to thermostat your system to compensate for energy changes resulting from broken bonds.

### Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes two statistics which it stores in a global vector of length 2, which can be accessed by various output commands. The vector values calculated by this fix are "intensive".

These are the 2 quantities:

- (1) # of bonds broken on the most recent breakage timestep
- (2) cumulative # of bonds broken

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

### Restrictions:

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Currently, there are 2 restrictions for using this fix. We may relax these in the future if there are new models that would be enabled by it.

When a bond is broken, you might wish to turn off angle and dihedral interactions that include that bond. However, LAMMPS does not check for these angles and dihedrals, even if your simulation defines an angle_style or dihedral_style.

This fix requires that the pairwise weightings defined by the special_bonds command be 0,1,1 for 1-2, 1-3, and 1-4 neighbors within the bond topology. This effectively means that the pairwise interaction between atoms I and J is turned off when a bond between them exists and will be turned on when the bond is broken. It also means that the pairwise interaction of I with J’s other bond partners is unaffected by the existence of the bond.

### Related commands:
fix bond/create, fix bond/swap, dump local, special_bonds

**Default:**

The option defaults are prob = 1.0.
fix bond/create command

Syntax:

fix ID group-ID bond/create Nevery itype jtype Rmin bondtype keyword values ...

- ID, group-ID are documented in fix command
- bond/create = style name of this fix command
- Nevery = attempt bond creation every this many steps
- itype,jtype = atoms of itype can bond to atoms of jtype
- Rmin = 2 atoms separated by less than Rmin can bond (distance units)
- bondtype = type of created bonds
- zero or more keyword/value pairs may be appended to args
- keyword = iparam or jparam or prob

iparam values = maxbond, newtype
  maxbond = max # of bonds of bondtype the itype atom can have
  newtype = change the itype atom to this type when maxbonds exist
jparam values = maxbond, newtype
  maxbond = max # of bonds of bondtype the jtype atom can have
  newtype = change the jtype atom to this type when maxbonds exist
prob values = fraction seed
  fraction = create a bond with this probability if otherwise eligible
  seed = random number seed (positive integer)

Examples:

fix 5 all bond/create 10 1 2 0.8 1
fix 5 all bond/create 1 3 3 0.8 1 prob 0.5 85784 iparam 2 3

Description:

Create bonds between pairs of atoms as a simulation runs according to specified criteria. This can be used to model cross-linking of polymers, the formation of a percolation network, etc. In this context, a bond means an interaction between a pair of atoms computed by the bond_style command. Once the bond is created it will be permanently in place. This is different than a pairwise bond-order potential such as Tersoff or AIREBO which infers bonds and many-body interactions based on the current geometry of a small cluster of atoms and effectively creates and destroys bonds from timestep to timestep as atoms move.

A check for possible new bonds is performed every Nevery timesteps. If two atoms I,J are within a distance Rmin of each other, if I is of atom type itype, if J is of atom type jtype, if both I and J are in the specified fix group, if a bond does not already exist between I and J, and if both I and J meet their respective maxbond requirement (explained below), then I,J is labeled as a "possible" bond pair.

If several atoms are close to an atom, it may have multiple possible bond partners. Every atom checks its list of possible bond partners and labels the closest such partner as its "sole" bond partner. After this is done, if atom I has atom J as its sole partner, and atom J has atom I as its sole partner, then the I,J bond is "eligible" to be formed.

Note that these rules mean an atom will only be part of at most one created bond on a given timestep. It also means that if atom I chooses atom J as its sole partner, but atom J chooses atom K is its sole partner (due to Rjk < Rij), then this means atom I will not form a bond on this timestep, even if it has other possible bond partners.
It is permissible to have itype = jtype. Rmin must be <= the pairwise cutoff distance between itype and jtype atoms, as defined by the pair_style command.

The iparam and jparam keywords can be used to limit the bonding functionality of the participating atoms. Each atom keeps track of how many bonds of bondtype it already has. If atom I of itype already has maxbond bonds (as set by the iparam keyword), then it will not form any more. Likewise for atom J. If maxbond is set to 0, then there is no limit on the number of bonds that can be formed with that atom.

The newtype value for iparam and jparam can be used to change the atom type of atom I or J when it reaches maxbond number of bonds of type bondtype. This means it can now interact in a pairwise fashion with other atoms in a different way by specifying different pair_coeff coefficients. If you do not wish the atom type to change, simply specify newtype as itype or jtype.

The prob keyword can also effect whether an eligible bond is actually created. The fraction setting must be a value between 0.0 and 1.0. A uniform random number between 0.0 and 1.0 is generated and the eligible bond is only created if the random number < fraction.

Any bond that is created is assigned a bond type of bondtype. Data structures within LAMMPS that store bond topology are updated to reflect the new bond. This can also affect subsequent computation of pairwise interactions involving the atoms in the bond. See the Restriction section below for additional information.

IMPORTANT NOTE: To create a new bond, the internal LAMMPS data structures that store this information must have space for it. When LAMMPS is initialized from a data file, the list of bonds is scanned and the maximum number of bonds per atom is tallied. If some atom will acquire more bonds than this limit as this fix operates, then the "extra bonds per atom" parameter in the data file header must be set to allow for it. See the read_data command for more details. Note that if this parameter needs to be set, it means a data file must be used to initialize the system, even if it initially has no bonds. A data file with no atoms can be used if you wish to add unbonded atoms via the create atoms command, e.g. for a percolation simulation.

IMPORTANT NOTE: LAMMPS also maintains a data structure that stores a list of 1st, 2nd, and 3rd neighbors of each atom (in the bond topology of the system) for use in weighting pairwise interactions for bonded atoms. Adding a bond adds a single entry to this list. The "extra" keyword of the special_bonds command should be used to leave space for new bonds if the maximum number of entries for any atom will be exceeded as this fix operates. See the special_bonds command for details.

Note that even if your simulation starts with no bonds, you must define a bond_style and use the bond_coeff command to specify coefficients for the bondtype. Similarly, if new atom types are specified by the iparam or jparam keywords, they must be within the range of atom types allowed by the simulation and pairwise coefficients must be specified for the new types.

Computationally, each timestep this fix operates, it loops over neighbor lists and computes distances between pairs of atoms in the list. It also communicates between neighboring processors to coordinate which bonds are created. Thus it roughly doubles the cost of a timestep. Thus you should be cautious about invoking this fix too frequently.

You can dump out snapshots of the current bond topology via the dump local command.

IMPORTANT NOTE: Creating a bond typically alters the energy of a system. You should be careful not to choose bond creation criteria that induce a dramatic change in energy. For example, if you define a very stiff harmonic bond and create it when 2 atoms are separated by a distance far from the equilibribum bond length, then the 2 atoms will oscillate dramatically when the bond is formed. More generally, you may need to thermostat your system to compensate for energy changes resulting from created bonds.
**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes two statistics which it stores in a global vector of length 2, which can be accessed by various output commands. The vector values calculated by this fix are "intensive".

These are the 2 quantities:

- (1) # of bonds created on the most recent creation timestep
- (2) cumulative # of bonds created

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Currently, there are 2 restrictions for using this fix. We may relax these in the future if there are new models that would be enabled by it.

When a bond is created, you might wish to induce new angle and dihedral interactions that include that bond. However, LAMMPS does not create these angles and dihedrals, even if your simulation defines an angle_style or dihedral_style.

This fix requires that the pairwise weightings defined by the special_bonds command be 0,1,1 for 1-2, 1-3, and 1-4 neighbors within the bond topology. This effectively means that the pairwise interaction between atoms I and J will be turned off when a bond between them is created. It also means that the pairwise interaction of I with J's other bond partners will be unaffected by the new bond.

**Related commands:**

fix bond/break, fix bond/swap, dump local, special_bonds

**Default:**

The option defaults are iparam = (0,itype), jparam = (0,jtype), and prob = 1.0.
fix bond/swap command

Syntax:

fix ID group-ID bond/swap fraction cutoff seed

- ID, group-ID are documented in fix command
- bond/swap = style name of this fix command
- fraction = fraction of group atoms to consider for swapping
- cutoff = distance at which swapping will be considered (distance units)
- seed = random # seed (positive integer)

Examples:

fix 1 all bond/swap 0.5 1.3 598934

Description:

In a simulation of polymer chains, this command attempts to swap bonds between two different chains, effectively grafting the end of one chain onto another chain and vice versa. This is done via Monte Carlo rules using the Boltzmann acceptance criterion. The purpose is to equilibrate the polymer chain conformations more rapidly than dynamics alone would do it, by enabling instantaneous large conformational changes in a dense polymer melt. The polymer chains should thus more rapidly converge to the proper end-to-end distances and radii of gyration. It is designed for use with systems of FENE or harmonic bead-spring polymer chains where each polymer is a linear chain of monomers, but LAMMPS does not enforce this requirement, i.e. any bond_style can be used.

A schematic of the kinds of bond swaps that can occur is shown here:

On the left, the red and blue chains have two monomers A1 and B1 close to each other, which are currently bonded to monomers A2 and B2 respectively within their own chains. The bond swap operation will attempt to delete the A1-A2 and B1-B2 bonds and replace them with A1-B2 and B1-A2 bonds. If the swap is energetically favorable, the two chains on the right are the result and each polymer chain has undergone a dramatic conformational change. This reference provides more details on how the algorithm works and its application: (Sides).

The bond swapping operation is invoked each time neighbor lists are built during a simulation, since it potentially alters the list of which neighbors are considered for pairwise interaction. At each reneighboring step, each processor considers a random specified fraction of its atoms as potential swapping monomers for this timestep. Choosing a small fraction value can reduce the likelihood of a reverse swap occurring soon after an initial swap.
For each monomer A1, its neighbors are examined to find a possible B1 monomer. Both A1 and B1 must be in the fix group, their separation must be less than the specified cutoff, and the molecule IDs of A1 and B1 must be the same (see below). If a suitable partner is found, the energy change due to swapping the 2 bonds is computed. This includes changes in pairwise, bond, and angle energies due to the altered connectivity of the 2 chains. Dihedral and improper interactions are not allowed to be defined when this fix is used.

If the energy decreases due to the swap operation, the bond swap is accepted. If the energy increases it is accepted with probability exp(-delta/kT) where delta is the increase in energy, k is the Boltzmann constant, and T is the current temperature of the system. Whether the swap is accepted or rejected, no other swaps are attempted by this processor on this timestep.

The criterion for matching molecule IDs is how bond swaps performed by this fix conserve chain length. To use this features you must setup the molecule IDs for your polymer chains in a certain way, typically in the data file, read by the read_data command. Consider a system of 6-mer chains. You have 2 choices. If the molecule IDs for monomers on each chain are set to 1,2,3,4,5,6 then swaps will conserve chain length. For a particular monomer there will be only one other monomer on another chain which is a potential swap partner. If the molecule IDs for monomers on each chain are set to 1,2,3,3,2,1 then swaps will conserve chain length but swaps will be able to occur at either end of a chain. Thus for a particular monomer there will be 2 possible swap partners on another chain. In this scenario, swaps can also occur within a single chain, i.e. the two ends of a chain swap with each other.

IMPORTANT NOTE: If your simulation uses molecule IDs in the usual way, where all monomers on a single chain are assigned the same ID (different for each chain), then swaps will only occur within the same chain. If you assign the same molecule ID to all monomers in all chains then inter-chain swaps will occur, but they will not conserve chain length. Neither of these scenarios is probably not what you want for this fix.

This fix computes a temperature each time it is invoked for use by the Boltzmann criterion. To do this, the fix creates its own compute of style temp, as if this command had been issued:

```
compute fix-ID_temp all temp
```

See the compute temp command for details. Note that the ID of the new compute is the fix-ID with underscore + "temp" appended and the group for the new compute is "all", so that the temperature of the entire system is used.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = thermo_temp. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of thermo_temp will have no effect on this fix.

**Restart, fix_modify, thermo output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior. Also note that each processor generates possible swaps independently of other processors. Thus if you repeat the same simulation on a different number of processors, the specific swaps performed will be different.

The fix_modify temp option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used to compute the temperature for the Boltzmann criterion.
This fix computes two statistical quantities as a global 2-vector of output, which can be accessed by various output commands. The first component of the vector is the cumulative number of swaps performed by all processors. The second component of the vector is the cumulative number of swaps attempted (whether accepted or rejected). Note that a swap "attempt" only occurs when swap partners meeting the criteria described above are found on a particular timestep. The vector values calculated by this fix are "intensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The settings of the "special_bond" command must be 0,1,1 in order to use this fix, which is typical of bead-spring chains with FENE or harmonic bonds. This means that pairwise interactions between bonded atoms are turned off, but are turned on between atoms two or three hops away along the chain backbone.

Currently, energy changes in dihedral and improper interactions due to a bond swap are not considered. Thus a simulation that uses this fix cannot use a dihedral or improper potential.

**Related commands:** none

**Default:** none

---

**fix box/relax command**

**Syntax:**

```
fix ID group-ID box/relax keyword value ...
```

- **ID, group-ID** are documented in the `fix` command
- **box/relax** = style name of this fix command
- one or more keyword value pairs may be appended
- keyword = `iso` or `aniso` or `tri` or `x` or `y` or `z` or `xy` or `yz` or `xz` or `couple` or `nreset` or `vmax` or `dilate`
- `iso` or `aniso` or `tri` value = `Ptarget` = desired pressure (pressure units)
- `x` or `y` or `z` or `xy` or `yz` or `xz` value = `Ptarget` = desired pressure (pressure units)
- `couple` = `none` or `xyz` or `xy` or `yz` or `xz`
- `nreset` value = reset reference cell every this many minimizer iterations
- `vmax` value = fraction = max allowed volume change in one iteration
- `dilate` value = `all` or `partial`
- `scaleyz` value = `yes` or `no` = scale `yz` with `lz`
- `scalexz` value = `yes` or `no` = scale `xz` with `lz`
- `scalexy` value = `yes` or `no` = scale `xy` with `ly`
- `fixedpoint` values = `x` `y` `z`
  - `x`, `y`, `z` = perform relaxation dilation/contraction around this point (distance units)

**Examples:**

```
fix 1 all box/relax iso 0.0 vmax 0.001
fix 2 water box/relax aniso 0.0 dilate partial
fix 2 ice box/relax tri 0.0 couple xy nreset 100
```

**Description:**

Apply an external pressure or stress tensor to the simulation box during an energy minimization. This allows the box size and shape to vary during the iterations of the minimizer so that the final configuration will be both an energy minimum for the potential energy of the atoms, and the system pressure tensor will be close to the specified external tensor. Conceptually, specifying a positive pressure is like squeezing on the simulation box; a negative pressure typically allows the box to expand.

The external pressure tensor is specified using one or more of the `iso`, `aniso`, `tri`, `x`, `y`, `z`, `xy`, `xz`, `yz`, and `couple` keywords. These keywords give you the ability to specify all 6 components of an external stress tensor, and to couple various of these components together so that the dimensions they represent are varied together during the minimization.

Orthogonal simulation boxes have 3 adjustable dimensions (`x`, `y`, `z`). Triclinic (non-orthogonal) simulation boxes have 6 adjustable dimensions (`x`, `y`, `z`, `xy`, `xz`, `yz`). The `create_box`, `read data`, and `read_restart` commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the `xy`, `xz`, `yz` tilt factors.

The target pressures `Ptarget` for each of the 6 components of the stress tensor can be specified independently via the `x`, `y`, `z`, `xy`, `xz`, `yz` keywords, which correspond to the 6 simulation box dimensions. For example, if the `y` keyword is used, the y-box length will change during the minimization. If the `xy` keyword is used, the `xy` tilt factor will change. A box dimension will not change if that component is not specified.
Note that in order to use the \(xy\), \(xz\), or \(yz\) keywords, the simulation box must be triclinic, even if its initial tilt factors are 0.0.

When the size of the simulation box changes, all atoms are re-scaled to new positions, unless the keyword \textit{dilate} is specified with a value of \textit{partial}, in which case only the atoms in the fix group are re-scaled. This can be useful for leaving the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

The \textit{scaleyz}, \textit{scalexz}, and \textit{scalexy} keywords control whether or not the corresponding tilt factors are scaled with the associated box dimensions when relaxing triclinic periodic cells. The default values \textit{yes} will turn on scaling, which corresponds to adjusting the linear dimensions of the cell while preserving its shape. Choosing \textit{no} ensures that the tilt factors are not scaled with the box dimensions. See below for restrictions and default values in different situations. In older versions of LAMMPS, scaling of tilt factors was not performed. The old behavior can be recovered by setting all three scale keywords to \textit{no}.

The \textit{fixedpoint} keyword specifies the fixed point for cell relaxation. By default, it is the center of the box. Whatever point is chosen will not move during the simulation. For example, if the lower periodic boundaries pass through \((0,0,0)\), and this point is provided to \textit{fixedpoint}, then the lower periodic boundaries will remain at \((0,0,0)\), while the upper periodic boundaries will move twice as far. In all cases, the particle positions at each iteration are unaffected by the chosen value, except that all particles are displaced by the same amount, different on each iteration.

\textbf{IMPORTANT NOTE:} Applying an external pressure to tilt dimensions \(xy\), \(xz\), \(yz\) can sometimes result in arbitrarily large values of the tilt factors, i.e. a dramatically deformed simulation box. This typically indicates that there is something badly wrong with how the simulation was constructed. The two most common sources of this error are applying a shear stress to a liquid system or specifying an external shear stress tensor that exceeds the yield stress of the solid. In either case the minimization may converge to a bogus conformation or not converge at all. Also note that if the box shape tilts to an extreme shape, LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

The \textit{couple} keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, \(xz\) means the \(P_{xx}\) and \(P_{zz}\) components of the stress tensor are coupled. \(xyz\) means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The \textit{Ptarget} values for any coupled dimensions must be identical. \textit{Couple xyz} can be used for a 2d simulation; the \(z\) dimension is simply ignored.

The \textit{iso}, \textit{aniso}, and \textit{tri} keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword \textit{iso} means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso \textit{Ptarget}" is the same as specifying these 4 keywords:

\begin{verbatim}
x \textit{Ptarget}
y \textit{Ptarget}
z \textit{Ptarget}
couple \textit{xyz}
\end{verbatim}

The keyword \textit{aniso} means \(x\), \(y\), and \(z\) dimensions are controlled independently using the \(P_{xx}\), \(P_{yy}\), and \(P_{zz}\) components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso
"Ptarget" is the same as specifying these 4 keywords:

- x Ptarget
- y Ptarget
- z Ptarget
- couple none

The keyword \texttt{tri} means $x$, $y$, $z$, $xy$, $xz$, and $yz$ dimensions are controlled independently using their individual stress components as the driving forces, and the specified scalar pressure as the external normal stress. Using "\texttt{tri Ptarget}" is the same as specifying these 7 keywords:

- x Ptarget
- y Ptarget
- z Ptarget
- xy 0.0
- yz 0.0
- xz 0.0
- couple none

The \texttt{vmax} keyword can be used to limit the fractional change in the volume of the simulation box that can occur in one iteration of the minimizer. If the pressure is not settling down during the minimization this can be because the volume is fluctuating too much. The specified fraction must be greater than 0.0 and should be $<< 1.0$. A value of 0.001 means the volume cannot change by more than 1/10 of a percent in one iteration when \texttt{couple xyz} has been specified. For any other case it means no linear dimension of the simulation box can change by more than 1/10 of a percent.

With this fix, the potential energy used by the minimizer is augmented by an additional energy provided by the fix. The overall objective function then is:

$$E = U + P_t (V - V_0) + E_{strain}$$

where $U$ is the system potential energy, $P_t$ is the desired hydrostatic pressure, $V$ and $V_0$ are the system and reference volumes, respectively. $E_{strain}$ is the strain energy expression proposed by Parrinello and Rahman (Parrinello1981). Taking derivatives of $E$ w.r.t. the box dimensions, and setting these to zero, we find that at the minimum of the objective function, the global system stress tensor $\mathbf{P}$ will satisfy the relation:

$$\mathbf{P} = P_t \mathbf{I} + S_t \left( \mathbf{h}_0^{-1} \right)^t \mathbf{h}_{0d}$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{h}_0$ is the box dimension tensor of the reference cell, and $\mathbf{h}_{0d}$ is the diagonal part of $\mathbf{h}_0$. $S_t$ is a symmetric stress tensor that is chosen by LAMMPS so that the upper-triangular components of $\mathbf{P}$ equal the stress tensor specified by the user.

This equation only applies when the box dimensions are equal to those of the reference dimensions. If this is not the case, then the converged stress tensor will not equal that specified by the user. We can resolve this problem by periodically resetting the reference dimensions. The keyword \texttt{nreset_ref} controls how often this is done. If this keyword is not used, or is given a value of zero, then the reference dimensions are set to those of the initial simulation domain and are never changed. A value of \texttt{nstep means that every nstep minimization steps, the}
reference dimensions are set to those of the current simulation domain. Note that resetting the reference dimensions changes the objective function and gradients, which sometimes causes the minimization to fail. This can be resolved by changing the value of nreset, or simply continuing the minimization from a restart file.

IMPORTANT NOTE: As normally computed, pressure includes a kinetic-energy or temperature-dependent component; see the compute pressure command. However, atom velocities are ignored during a minimization, and the applied pressure(s) specified with this command are assumed to only be the virial component of the pressure (the non-kinetic portion). Thus if atoms have a non-zero temperature and you print the usual thermodynamic pressure, it may not appear the system is converging to your specified pressure. The solution for this is to either (a) zero the velocities of all atoms before performing the minimization, or (b) make sure you are monitoring the pressure without its kinetic component. The latter can be done by outputting the pressure from the fix this command creates (see below) or a pressure fix you define yourself.

IMPORTANT NOTE: Because pressure is often a very sensitive function of volume, it can be difficult for the minimizer to equilibrate the system the desired pressure with high precision, particularly for solids. Some techniques that seem to help are (a) use the "min_modify line quadratic" option when minimizing with box relaxations, and (b) minimize several times in succession if need be, to drive the pressure closer to the target pressure. Also note that some systems (e.g. liquids) will not sustain a non-hydrostatic applied pressure, which means the minimizer will not converge.

This fix computes a temperature and pressure each timestep. The temperature is used to compute the kinetic contribution to the pressure, even though this is subsequently ignored by default. To do this, the fix creates its own computes of style "temp" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp virial
```

See the compute temp and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is the same as the fix group. Also note that the pressure compute does not include a kinetic component.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = thermo_temp and thermo_press. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of thermo_temp or thermo_press will have no effect on this fix.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify temp and press options are supported by this fix. You can use them to assign a compute you have defined to this fix which will be used in its temperature and pressure calculation, as described above. Note that as described above, if you assign a pressure compute to this fix that includes a kinetic energy component it will affect the minimization, most likely in an undesirable way.

IMPORTANT NOTE: If both the temp and press keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a pressure compute defines its own temperature compute as an argument when it is specified. The temp keyword will override this (for the pressure compute being used by fix npt), but only if the temp keyword comes after the press keyword. If the temp keyword comes before the press keyword, then the new pressure compute specified by the press keyword will be unaffected by the temp setting.
This fix computes a global scalar which can be accessed by various output commands. The scalar is the pressure-volume energy, plus the strain energy, if it exists.

No parameter of this fix can be used with the start/stop keywords of the run command.

This fix is invoked during energy minimization, but not for the purpose of adding a contribution to the energy or forces being minimized. Instead it alters the simulation box geometry as described above.

**Restrictions:**

Only dimensions that are available can be adjusted by this fix. Non-periodic dimensions are not available. z, xz, and yz, are not available for 2D simulations. xy, xz, and yz are only available if the simulation domain is non-orthogonal. The create_box, read data, and read_restart commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

The scaleyz yes and scalexz yes keyword/value pairs can not be used for 2D simulations. scaleyz yes, scalexz yes, and scalexy yes options can only be used if the 2nd dimension in the keyword is periodic, and if the tilt factor is not coupled to the barostat via keywords tri, yz, xz, and xy.

**Related commands:**

fix npt, minimize

**Default:**

The keyword defaults are dilate = all, vmax = 0.0001, nreset = 0.

---

fix colvars command

Syntax:

fix ID group-ID colvars configfile keyword values ...

- ID, group-ID are documented in fix command
- colvars = style name of this fix command
- configfile = the configuration file for the colvars module
- keyword = input or output or seed or tstat

input arg = colvars.state file name or prefix or NULL (default: NULL)
output arg = output filename prefix (default: out)
seed arg = seed for random number generator (default: 1966)
tstat arg = fix id of a thermostat or NULL (default: NULL)

Examples:

fix colvars peptide peptide.colvars.inp seed 2122 input peptide.colvars.state output peptide
fix colvars all colvars.inp

Description:

This fix interfaces LAMMPS to a "collective variables" or "colvars" module library which allows to calculate potentials of mean force (PMFs) for any set of colvars, using different sampling methods: currently implemented are the Adaptive Biasing Force (ABF) method, metadynamics, Steered Molecular Dynamics (SMD) and Umbrella Sampling (US) via a flexible harmonic restraint bias. This documentation describes only the colvars fix itself and LAMMPS specific parts of the code. The documentation of the colvars implementation itself is available as part of the NAMD online documentation

There are example scripts for using this package with LAMMPS in examples/USER/colvars.

The implementation of the portable collective variable library is also documented in (Henin)

The only mandatory argument to the fix is the filename to the colvars input file that contains all input that is independent from the MD program in which the colvars library has been integrated.

The group-ID entry is ignored. The collective variable module will always apply to the entire system, i.e. use the group all.

The input keyword allows to specify a state file that would contain the information required in order to continue a calculation, e.g. from a restart. Setting it to NULL will start a new colvars run.

The output keyword allows to specify the output prefix. All output files generated will use this prefix followed by the ".colvars." and a word like "state" or "traj".

The seed keyword contains the seed for the random number generator that will be used in the colvars module.

The tstat keyword can be either NULL or the label of a thermostating fix that thermostats all atoms in the fix colvars group. This will be used to provide the colvars module with the current thermostat target temperature.
Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify energy option is supported by this fix to add the energy change from the biasing force added by the fix to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

Restrictions:

This fix is part of the USER-COLVARS package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

There can only be one colvars fix active at a time. Since the colvars module itself can handle an arbitrary number of collective variables and always applies to the entire system, this is not really a deficit in practice.

Related commands:

fix smd

Default:

The default options are input = NULL, output = out, seed = 1966, and tstat = NULL.

**fix deform command**

**Syntax:**

\[ \text{fix ID group-ID deform N parameter args ... keyword value ...} \]

- **ID, group-ID** are documented in **fix command**
- **deform** = style name of this fix command
- **N** = perform box deformation every this many timesteps
- one or more parameter/arg pairs may be appended

\[ \text{parameter} = \text{x or y or z or xy or xz or yz} \]

\[ x, y, z \text{ args} = \text{style value(s)} \]

\[ \text{style} = \text{final or delta or scale or vel or erate or trate or volume or wiggle or variable} \]

\[ \text{final values} = \text{lo hi} \]

\[ \text{lo hi} = \text{box boundaries at end of run (distance units)} \]

\[ \text{delta values} = \text{dlo dhi} \]

\[ \text{dlo dhi} = \text{change in box boundaries at end of run (distance units)} \]

\[ \text{scale values} = \text{factor} \]

\[ \text{factor} = \text{multiplicative factor for change in box length at end of run} \]

\[ \text{vel value} = V \]

\[ V = \text{change box length at this velocity (distance/time units), effectively an engineering strain rate} \]

\[ \text{erate value} = R \]

\[ R = \text{engineering strain rate (1/time units)} \]

\[ \text{trate value} = R \]

\[ R = \text{true strain rate (1/time units)} \]

\[ \text{volume value} = \text{none} = \text{adjust this dim to preserve volume of system} \]

\[ \text{wiggle values} = A Tp \]

\[ A = \text{amplitude of oscillation (distance units)} \]

\[ Tp = \text{period of oscillation (time units)} \]

\[ \text{variable values} = \text{v_name1 v_name2} \]

\[ \text{v_name1} = \text{variable with name1 for box length change as function of time} \]

\[ \text{v_name2} = \text{variable with name2 for change rate as function of time} \]

\[ \text{xy, xz, yz args} = \text{style value} \]

\[ \text{style} = \text{final or delta or vel or erate or trate or wiggle} \]

\[ \text{final value} = \text{tilt} \]

\[ \text{tilt} = \text{tilt factor at end of run (distance units)} \]

\[ \text{delta value} = \text{dtilt} \]

\[ \text{dtilt} = \text{change in tilt factor at end of run (distance units)} \]

\[ \text{vel value} = V \]

\[ V = \text{change tilt factor at this velocity (distance/time units), effectively an engineering shear strain rate} \]

\[ \text{erate value} = R \]

\[ R = \text{engineering shear strain rate (1/time units)} \]

\[ \text{trate value} = R \]

\[ R = \text{true shear strain rate (1/time units)} \]

\[ \text{wiggle values} = A Tp \]

\[ A = \text{amplitude of oscillation (distance units)} \]

\[ Tp = \text{period of oscillation (time units)} \]

\[ \text{variable values} = \text{v_name1 v_name2} \]

\[ \text{v_name1} = \text{variable with name1 for tilt change as function of time} \]

\[ \text{v_name2} = \text{variable with name2 for change rate as function of time} \]

- zero or more keyword/value pairs may be appended
- **keyword** = **remap or flip or units**

\[ \text{remap value} = \text{x or v or none} \]

\[ x = \text{remap coords of atoms in group into deforming box} \]
v = remap velocities of all atoms when they cross periodic boundaries
none = no remapping of x or v
flip value = yes or no
allow or disallow box flips when it becomes highly skewed
units value = lattice or box
  lattice = distances are defined in lattice units
  box = distances are defined in simulation box units

Examples:

fix 1 all deform 1 x final 0.0 9.0 z final 0.0 5.0 units box
fix 1 all deform 1 x trate 0.1 y volume z volume
fix 1 all deform 1 xy erate 0.001 remap v
fix 1 all deform 10 y delta -0.5 0.5 xz vel 1.0

Description:

Change the volume and/or shape of the simulation box during a dynamics run. Orthogonal simulation boxes have 3 adjustable parameters (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable parameters (x,y,z,xy,xz,yz). Any or all of them can be adjusted independently and simultaneously by this command. This fix can be used to perform non-equilibrium MD (NEMD) simulations of a continuously strained system. See the fix nvt/sllod and compute temp/deform commands for more details.

For the x, y, z parameters, the associated dimension cannot be shrink-wrapped. For the xy, yz, xz parameters, the associated 2nd dimension cannot be shrink-wrapped. Dimensions not varied by this command can be periodic or non-periodic. Dimensions corresponding to unspecified parameters can also be controlled by a fix npt or fix nph command.

The size and shape of the simulation box at the beginning of the simulation run were either specified by the create_box or read_data or read_restart command used to setup the simulation initially if it is the first run, or they are the values from the end of the previous run. The create_box, read data, and read_restart commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors. If fix deform changes the xy,xz,yz tilt factors, then the simulation box must be triclinic, even if its initial tilt factors are 0.0.

As described below, the desired simulation box size and shape at the end of the run are determined by the parameters of the fix deform command. Every Nth timestep during the run, the simulation box is expanded, contracted, or tilted to ramped values between the initial and final values.

For the x, y, and z parameters, this is the meaning of their styles and values.

The final, delta, scale, vel, and erate styles all change the specified dimension of the box via "constant displacement" which is effectively a "constant engineering strain rate". This means the box dimension changes linearly with time from its initial to final value.

For style final, the final lo and hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style delta, plus or minus changes in the lo/hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style scale, a multiplicative factor to apply to the box length of a dimension is specified. For example, if the initial box length is 10, and the factor is 1.1, then the final box length will be 11. A factor less than 1.0 means compression.
For style *vel*, a velocity at which the box length changes is specified in units of distance/time. This is effectively a "constant engineering strain rate", where rate = \( V/L_0 \) and \( L_0 \) is the initial box length. The distance can be in lattice or box distance units. See the discussion of the units keyword below. For example, if the initial box length is 100 Angstroms, and \( V \) is 10 Angstroms/psec, then after 10 psec, the box length will have doubled. After 20 psec, it will have tripled.

The *erate* style changes a dimension of the the box at a "constant engineering strain rate". The units of the specified strain rate are 1/time. See the units command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Tensile strain is unitless and is defined as \( \delta/\delta_0 \), where \( \delta_0 \) is the original box length and \( \delta \) is the change relative to the original length. The box length \( L \) as a function of time will change as

\[
L(t) = L_0 (1 + erate*dt)
\]

where \( dt \) is the elapsed time (in time units). Thus if *erate* \( R \) is specified as 0.1 and time units are picoseconds, this means the box length will increase by 10\% of its original length every picosecond. I.e. strain after 1 psec = 0.1, strain after 2 psec = 0.2, etc. \( R = -0.01 \) means the box length will shrink by 1\% of its original length every picosecond. Note that for an "engineering" rate the change is based on the original box length, so running with \( R = 1 \) for 10 picoseconds expands the box length by a factor of 11 (strain of 10), which is different that what the *trate* style would induce.

The *trate* style changes a dimension of the box at a "constant true strain rate". Note that this is not an "engineering strain rate", as the other styles are. Rather, for a "true" rate, the rate of change is constant, which means the box dimension changes non-linearly with time from its initial to final value. The units of the specified strain rate are 1/time. See the units command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Tensile strain is unitless and is defined as \( \delta/\delta_0 \), where \( \delta_0 \) is the original box length and \( \delta \) is the change relative to the original length.

The box length \( L \) as a function of time will change as

\[
L(t) = L_0 \exp(trate*dt)
\]

where \( dt \) is the elapsed time (in time units). Thus if *trate* \( R \) is specified as \( \ln(1.1) \) and time units are picoseconds, this means the box length will increase by 10\% of its current (not original) length every picosecond. I.e. strain after 1 psec = 0.1, strain after 2 psec = 0.21, etc. \( R = \ln(2) \) or \( \ln(3) \) means the box length will double or triple every picosecond. \( R = \ln(0.99) \) means the box length will shrink by 1\% of its current length every picosecond. Note that for a "true" rate the change is continuous and based on the current length, so running with \( R = \ln(2) \) for 10 picoseconds does not expand the box length by a factor of 11 as it would with *erate*, but by a factor of 1024 since the box length will double every picosecond.

Note that to change the volume (or cross-sectional area) of the simulation box at a constant rate, you can change multiple dimensions via *erate* or *trate*. E.g. to double the box volume in a picosecond picosecond, you could set "x erate M", "y erate M", "z erate M", with \( M = \text{pow}(2,1/3) - 1 = 0.26 \), since if each box dimension grows by 26\%, the box volume doubles. Or you could set "x trate M", "y trate M", "z trate M", with \( M = \ln(1.26) = 0.231 \), and the box volume would double every picosecond.

The *volume* style changes the specified dimension in such a way that the box volume remains constant while other box dimensions are changed explicitly via the styles discussed above. For example, "x scale 1.1 y scale 1.1 z volume" will shrink the z box length as the x,y box lengths increase, to keep the volume constant (product of x,y,z lengths). If "x scale 1.1 z volume" is specified and parameter y is unspecified, then the z box length will shrink as x increases to keep the product of x,z lengths constant. If "x scale 1.1 y volume z volume" is specified, then both the y,z box lengths will shrink as x increases to keep the volume constant (product of x,y,z lengths). In this case, the y,z box lengths shrink so as to keep their relative aspect ratio constant.
For solids or liquids, note that when one dimension of the box is expanded via fix deform (i.e. tensile strain), it may be physically undesirable to hold the other 2 box lengths constant (unspecified by fix deform) since that implies a density change. Using the *volume* style for those 2 dimensions to keep the box volume constant may make more physical sense, but may also not be correct for materials and potentials whose Poisson ratio is not 0.5. An alternative is to use *fix npt aniso* with zero applied pressure on those 2 dimensions, so that they respond to the tensile strain dynamically.

The *wiggle* style oscillates the specified box length dimension sinusoidally with the specified amplitude and period. I.e. the box length \( L \) as a function of time is given by

\[
L(t) = L_0 + A \sin(2\pi t/T_p)
\]

where \( L_0 \) is its initial length. If the amplitude \( A \) is a positive number the box initially expands, then contracts, etc. If \( A \) is negative then the box initially contracts, then expands, etc. The amplitude can be in lattice or box distance units. See the discussion of the units keyword below.

The *variable* style changes the specified box length dimension by evaluating a variable, which presumably is a function of time. The variable with \( name1 \) must be an equal-style variable and should calculate a change in box length in units of distance. Note that this distance is in box units, not lattice units; see the discussion of the *units* keyword below. The formula associated with variable \( name1 \) can reference the current timestep. Note that it should return the "change" in box length, not the absolute box length. This means it should evaluate to 0.0 when invoked on the initial timestep of the run following the definition of fix deform. It should evaluate to a value > 0.0 to dilate the box at future times, or a value < 0.0 to compress the box.

The variable \( name2 \) must also be an equal-style variable and should calculate the rate of box length change, in units of distance/time, i.e. the time-derivative of the \( name1 \) variable. This quantity is used internally by LAMMPS to reset atom velocities when they cross periodic boundaries. It is computed internally for the other styles, but you must provide it when using an arbitrary variable.

Here is an example of using the *variable* style to perform the same box deformation as the *wiggle* style formula listed above, where we assume that the current timestep = 0.

```plaintext
variable A equal 5.0
variable Tp equal 10.0
variable displace equal "v_A * sin(2*PI * step*dt/v_Tp)"
variable rate equal "2*PI*v_A/v_Tp * cos(2*PI * step*dt/v_Tp)"
fix 2 all deform 1 x variable v_displace v_rate remap v
```

For the *scale*, *vel*, *erate*, *trate*, *volume*, *wiggle*, and *variable* styles, the box length is expanded or compressed around its mid point.

For the \( xy, xz, \) and \( yz \) parameters, this is the meaning of their styles and values. Note that changing the tilt factors of a triclinic box does not change its volume.

The *final*, *delta*, *vel*, and *erate* styles all change the shear strain at a "constant engineering shear strain rate". This means the tilt factor changes linearly with time from its initial to final value.

For style *final*, the final tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

For style *delta*, a plus or minus change in the tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.
For style *vel*, a velocity at which the tilt factor changes is specified in units of distance/time. This is effectively an "engineering shear strain rate", where rate = V/L0 and L0 is the initial box length perpendicular to the direction of shear. The distance can be in lattice or box distance units. See the discussion of the units keyword below. For example, if the initial tilt factor is 5 Angstroms, and the V is 10 Angstroms/psec, then after 1 psec, the tilt factor will be 15 Angstroms. After 2 psec, it will be 25 Angstroms.

The *erate* style changes a tilt factor at a "constant engineering shear strain rate". The units of the specified shear strain rate are 1/time. See the units command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Shear strain is unitless and is defined as offset/length, where length is the box length perpendicular to the shear direction (e.g. y box length for xy deformation) and offset is the displacement distance in the shear direction (e.g. x direction for xy deformation) from the unstrained orientation.

The tilt factor T as a function of time will change as

\[ T(t) = T_0 + L_0 \times erate \times dt \]

where \( T_0 \) is the initial tilt factor, \( L_0 \) is the original length of the box perpendicular to the shear direction (e.g. y box length for xy deformation), and \( dt \) is the elapsed time (in time units). Thus if \( erate \) R is specified as 0.1 and time units are picoseconds, this means the shear strain will increase by 0.1 every picosecond. i.e. if the xy shear strain was initially 0.0, then strain after 1 psec = 0.1, strain after 2 psec = 0.2, etc. Thus the tilt factor would be 0.0 at time 0, 0.1*xybox at 1 psec, 0.2*xybox at 2 psec, etc, where xybox is the original y box length. R = 1 or 2 means the tilt factor will increase by 1 or 2 every picosecond. R = -0.01 means a decrease in shear strain by 0.01 every picosecond.

The *trate* style changes a tilt factor at a "constant true shear strain rate". Note that this is not an "engineering shear strain rate", as the other styles are. Rather, for a "true" rate, the rate of change is constant, which means the tilt factor changes non-linearly with time from its initial to final value. The units of the specified shear strain rate are 1/time. See the units command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Shear strain is unitless and is defined as offset/length, where length is the box length perpendicular to the shear direction (e.g. y box length for xy deformation) and offset is the displacement distance in the shear direction (e.g. x direction for xy deformation) from the unstrained orientation.

The tilt factor T as a function of time will change as

\[ T(t) = T_0 \exp(trate \times dt) \]

where \( T_0 \) is the initial tilt factor and \( dt \) is the elapsed time (in time units). Thus if \( trate \) R is specified as \( \ln(1.1) \) and time units are picoseconds, this means the shear strain or tilt factor will increase by 10% every picosecond. i.e. if the xy shear strain was initially 0.1, then strain after 1 psec = 0.11, strain after 2 psec = 0.121, etc. R = \( \ln(2) \) or \( \ln(3) \) means the tilt factor will double or triple every picosecond. R = \( \ln(0.99) \) means the tilt factor will shrink by 1% every picosecond. Note that the change is continuous, so running with R = \( \ln(2) \) for 10 picoseconds does not change the tilt factor by a factor of 10, but by a factor of 1024 since it doubles every picosecond. Note that the initial tilt factor must be non-zero to use the *trate* option.

Note that shear strain is defined as the tilt factor divided by the perpendicular box length. The *erate* and *trate* styles control the tilt factor, but assume the perpendicular box length remains constant. If this is not the case (e.g. it changes due to another fix deform parameter), then this effect on the shear strain is ignored.

The *wiggle* style oscillates the specified tilt factor sinusoidally with the specified amplitude and period. i.e. the tilt factor T as a function of time is given by

\[ T(t) = T_0 + A \sin(2\pi t/T_p) \]
where T0 is its initial value. If the amplitude A is a positive number the tilt factor initially becomes more positive, then more negative, etc. If A is negative then the tilt factor initially becomes more negative, then more positive, etc. The amplitude can be in lattice or box distance units. See the discussion of the units keyword below.

The variable style changes the specified tilt factor by evaluating a variable, which presumably is a function of time. The variable with name1 must be an equal-style variable and should calculate a change in tilt in units of distance. Note that this distance is in box units, not lattice units; see the discussion of the units keyword below. The formula associated with variable name1 can reference the current timestep. Note that it should return the "change" in tilt factor, not the absolute tilt factor. This means it should evaluate to 0.0 when invoked on the initial timestep of the run following the definition of fix deform.

The variable name2 must also be an equal-style variable and should calculate the rate of tilt change, in units of distance/time, i.e. the time-derivative of the name1 variable. This quantity is used internally by LAMMPS to reset atom velocities when they cross periodic boundaries. It is computed internally for the other styles, but you must provide it when using an arbitrary variable.

Here is an example of using the variable style to perform the same box deformation as the wiggle style formula listed above, where we assume that the current timestep = 0.

```
variable A equal 5.0
variable Tp equal 10.0
variable displace equal "v_A * sin(2*PI * step*dt/v_Tp)"
variable rate equal "2*PI*v_A/v_Tp * cos(2*PI * step*dt/v_Tp)"
fix 2 all deform 1 xy variable v_displace v_rate remap v
```

All of the tilt styles change the xy, xz, yz tilt factors during a simulation. In LAMMPS, tilt factors (xy,xz,yz) for triclinic boxes are normally bounded by half the distance of the parallel box length. See the discussion of the flip keyword below, to allow this bound to be exceeded, if desired.

For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all equivalent.

To obey this constraint and allow for large shear deformations to be applied via the xy, xz, or yz parameters, the following algorithm is used. If prd is the associated parallel box length (10 in the example above), then if the tilt factor exceeds the accepted range of -5 to 5 during the simulation, then the box is flipped to the other limit (an equivalent box) and the simulation continues. Thus for this example, if the initial xy tilt factor was 0.0 and "xy final 100.0" was specified, then during the simulation the xy tilt factor would increase from 0.0 to 5.0, the box would be flipped so that the tilt factor becomes -5.0, the tilt factor would increase from -5.0 to 5.0, the box would be flipped again, etc. The flip occurs 10 times and the final tilt factor at the end of the simulation would be 0.0. During each flip event, atoms are remapped into the new box in the appropriate manner.

The one exception to this rule is if the 1st dimension in the tilt factor (x for xy) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient due to the highly skewed simulation box.

Each time the box size or shape is changed, the remap keyword determines whether atom positions are remapped to the new box. If remap is set to x (the default), atoms in the fix group are remapped; otherwise they are not. Note that their velocities are not changed, just their positions are altered. If remap is set to v, then any atom in the fix group that crosses a periodic boundary will have a delta added to its velocity equal to the difference in velocities between the lo and hi boundaries. Note that this velocity difference can include tilt components, e.g. a
delta in the x velocity when an atom crosses the y periodic boundary. If remap is set to none, then neither of these remappings take place.

Conceptually, setting remap to x forces the atoms to deform via an affine transformation that exactly matches the box deformation. This setting is typically appropriate for solids. Note that though the atoms are effectively "moving" with the box over time, it is not due to their having a velocity that tracks the box change, but only due to the remapping. By contrast, setting remap to v is typically appropriate for fluids, where you want the atoms to respond to the change in box size/shape on their own and acquire a velocity that matches the box change, so that their motion will naturally track the box without explicit remapping of their coordinates.

IMPORTANT NOTE: When non-equilibrium MD (NEMD) simulations are performed using this fix, the option "remap v" should normally be used. This is because fix nvt/sllod adjusts the atom positions and velocities to induce a velocity profile that matches the changing box size/shape. Thus atom coordinates should NOT be remapped by fix deform, but velocities SHOULD be when atoms cross periodic boundaries, since that is consistent with maintaining the velocity profile already created by fix nvt/sllod. LAMMPS will warn you if the remap setting is not consistent with fix nvt/sllod.

IMPORTANT NOTE: If a fix rigid is defined for rigid bodies, and remap is set to x, then the center-of-mass coordinates of rigid bodies will be remapped to the changing simulation box. This will be done regardless of whether atoms in the rigid bodies are in the fix deform group or not. The velocity of the centers of mass are not remapped even if remap is set to v, since fix nvt/sllod does not currently do anything special for rigid particles. If you wish to perform a NEMD simulation of rigid particles, you can either thermostat them independently or include a background fluid and thermostat the fluid via fix nvt/sllod.

The flip keyword allows the tilt factors for a triclinic box to exceed half the distance of the parallel box length, as discussed above. If the flip value is set to yes, the bound is enforced by flipping the box when it is exceeded. If the flip value is set to no, the tilt will continue to change without flipping. Note that if you apply large deformations, this means the box shape can tilt dramatically LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

The units keyword determines the meaning of the distance units used to define various arguments. A box value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A lattice value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. Note that the units choice also affects the vel style parameters since it is defined in terms of distance/time. Also note that the units keyword does not affect the variable style. You should use the xlat, ylat, zlat keywords of the thermo_style command if you want to include lattice spacings in a variable formula.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands.

This fix can perform deformation over multiple runs, using the start and stop keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

You cannot apply x, y, or z deformations to a dimension that is shrink-wrapped via the boundary command.
You cannot apply xy, yz, or xz deformations to a 2nd dimension (y in xy) that is shrink-wrapped via the boundary command.

Related commands:

change_box

Default:

The option defaults are remap = x, flip = yes, and units = lattice.
fix deposit command

Syntax:

fix ID group-ID deposit N type M seed keyword values ...

- ID, group-ID are documented in fix command
- deposit = style name of this fix command
- N = # of atoms to insert
- type = atom type to assign to inserted atoms
- M = insert a single particle every M steps
- seed = random # seed (positive integer)
- one or more keyword/value pairs may be appended to args
- keyword = region or global or local or near or attempt or rate or vx or vy or vz or units

region value = region-ID
  region-ID = ID of region to use as insertion volume

global values = lo hi
  lo, hi = put new particle a distance lo-hi above all other particles (distance units)

local values = lo hi delta
  lo, hi = put new particle a distance lo-hi above any nearby particle beneath it (distance units)
  delta = lateral distance within which a neighbor is considered "nearby" (distance units)

near value = R
  R = only insert particle if further than R from existing particles (distance units)

attempt value = Q
  Q = attempt a single insertion up to Q times

rate value = V
  V = z velocity (y in 2d) at which insertion volume moves (velocity units)

vx values = vxlo vxhi
  vxlo, vxhi = range of x velocities for inserted particle (velocity units)

vy values = vylo vyhi
  vylo, vyhi = range of y velocities for inserted particle (velocity units)

vz values = vzlo vzhi
  vzlo, vzhi = range of z velocities for inserted particle (velocity units)

target values = tx ty tz
  tx, ty, tz = location of sputtering target (distance units)

units value = lattice or box
  lattice = the geometry is defined in lattice units
  box = the geometry is defined in simulation box units

Examples:

fix 3 all deposit 1000 2 100 29494 region myblock local 1.0 1.0 1.0 units box
fix 2 newatoms deposit 10000 1 500 12345 region disk near 2.0 vz -1.0 -0.8

fix 4 sputter deposit 1000 2 500 12235 region sphere vz -1.0 -1.0 target 5.0 5.0 0.0 units lattice

Description:

Insert a single particle into the simulation domain every M timesteps until N particles have been inserted. This is useful for simulating the deposition of particles onto a surface.

Inserted particles have the specified atom type and are assigned to two groups: the default group "all" and the group specified in the fix deposit command (which can also be "all").
If you are computing temperature values which include inserted particles, you will want to use the `compute_modify` dynamic option, which insures the current number of atoms is used as a normalizing factor each time temperature is computed.

Care must be taken that inserted particles are not too near existing particles, using the options described below. When inserting particles above a surface in a non-periodic box (see the `boundary` command), the possibility of a particle escaping the surface and flying upward should be considered, since the particle may be lost or the box size may grow infinitely large. A `fix wall/reflect` command can be used to prevent this behavior. Note that if a shrink-wrap boundary is used, it is OK to insert the new particle outside the box, however the box will immediately be expanded to include the new particle. When simulating a sputtering experiment it is probably more realistic to ignore those atoms using the `thermo_modify` command with the `lost ignore` option and a fixed boundary.

This command must use the `region` keyword to define an insertion volume. The specified region must have been previously defined with a `region` command. It must be defined with side = `in`.

Each timestep a particle is to be inserted, its coordinates are chosen as follows. A random position within the insertion volume is generated. If neither the `global` or `local` keyword is used, that is the trial position. If the `global` keyword is used, the random x,y values are used, but the z position of the new particle is set above the highest current atom in the simulation by a distance randomly chosen between lo/hi. (For a 2d simulation, this is done for the y position.) If the `local` keyword is used, the z position is set a distance between lo/hi above the highest current atom in the simulation that is "nearby" the chosen x,y position. In this context, "nearby" means the lateral distance (in x,y) between the new and old particles is less than the delta parameter.

Once a trial x,y,z location has been computed, the insertion is only performed if no current particle in the simulation is within a distance R of the new particle. If this test fails, a new random position within the insertion volume is chosen and another trial is made. Up to Q attempts are made. If an atom is not successfully deposited, LAMMPS prints a warning message.

The `rate` option moves the insertion volume in the z direction (3d) or y direction (2d). This enables particles to be inserted from a successively higher height over time. Note that this parameter is ignored if the `global` or `local` keywords are used, since those options choose a z-coordinate for insertion independently.

The vx, vy, and vz components of velocity for the inserted particle are set using the values specified for the `vx`, `vy`, and `vz` keywords. Note that normally, new particles should be assigned a negative vertical velocity so that they move towards the surface.

In case the `target` option is used, the velocity vector of the inserted particle will be changed in a way so that it would pass through the specified coordinate. This allows convenient simulation of a sputtering process.

The `units` keyword determines the meaning of the distance units used for the other deposition parameters. A `box` value selects standard distance units as defined by the `units` command, e.g. Angstroms for units = real or metal. A `lattice` value means the distance units are in lattice spacings. The `lattice` command must have been previously used to define the lattice spacing. Note that the units choice affects all the keyword values that have units of distance or velocity.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the state of the deposition to binary restart files. This includes information about how many atoms have been deposited, the random number generator seed, the next timestep for deposition, etc. See the `read_restart` command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.
None of the `fix_modify` options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various `output commands`. No parameter of this fix can be used with the `start/stop` keywords of the `run` command. This fix is not invoked during `energy minimization`.

**Restrictions:**

The specified insertion region cannot be a "dynamic" region, as defined by the `region` command.

**Related commands:**

`fix_pour, region`

**Default:**

The option defaults are `delta = 0.0, near = 0.0, attempt = 10, rate = 0.0, vx = 0.0 0.0, vy = 0.0 0.0, vz = 0.0 0.0,` and `units = lattice.`
**fix drag command**

**Syntax:**

```
fix ID group-ID drag x y z fmag delta
```

- ID, group-ID are documented in fix command
- drag = style name of this fix command
- x,y,z = coord to drag atoms towards
- fmag = magnitude of force to apply to each atom (force units)
- delta = cutoff distance inside of which force is not applied (distance units)

**Examples:**

```
fix center small-molecule drag 0.0 10.0 0.0 5.0 2.0
```

**Description:**

Apply a force to each atom in a group to drag it towards the point (x,y,z). The magnitude of the force is specified by fmag. If an atom is closer than a distance delta to the point, then the force is not applied.

Any of the x,y,z values can be specified as NULL which means do not include that dimension in the distance calculation or force application.

This command can be used to steer one or more atoms to a new location in the simulation.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various output commands. This is the total force on the group of atoms by the drag force. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

fix spring, fix spring/self, fix spring/rg, fix smd

**Default:** none
fix dt/reset command

Syntax:

fix ID group-ID dt/reset N Tmin Tmax Xmax keyword values ...

- ID, group-ID are documented in fix command
- dt/reset = style name of this fix command
- N = recompute dt every N timesteps
- Tmin = minimum dt allowed which can be NULL (time units)
- Tmax = maximum dt allowed which can be NULL (time units)
- Xmax = maximum distance for an atom to move in one timestep (distance units)
- zero or more keyword/value pairs may be appended
- keyword = units

units value = lattice or box
  lattice = Xmax is defined in lattice units
  box = Xmax is defined in simulation box units

Examples:

fix 5 all dt/reset 10 1.0e-5 0.01 0.1
fix 5 all dt/reset 10 0.01 2.0 0.2 units box

Description:

Reset the timestep size every N steps during a run, so that no atom moves further than Xmax, based on current atom velocities and forces. This can be useful when starting from a configuration with overlapping atoms, where forces will be large. Or it can be useful when running an impact simulation where one or more high-energy atoms collide with a solid, causing a damage cascade.

This fix overrides the timestep size setting made by the timestep command. The new timestep size dt is computed in the following manner.

For each atom, the timestep is computed that would cause it to displace Xmax on the next integration step, as a function of its current velocity and force. Since performing this calculation exactly would require the solution to a quartic equation, a cheaper estimate is generated. The estimate is conservative in that the atom's displacement is guaranteed not to exceed Xmax, though it may be smaller.

Given this putative timestep for each atom, the minimum timestep value across all atoms is computed. Then the Tmin and Tmax bounds are applied, if specified. If one (or both) is specified as NULL, it is not applied.

When the run style is respa, this fix resets the outer loop (largest) timestep, which is the same timestep that the timestep command sets.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.
This fix computes a global scalar and a global vector of length 2, which can be accessed by various output commands. The scalar is the current timestep size.

The first element of the vector stores the cumulative simulation time (in time units). The cumulative time is zeroed when the fix is created and continuously accrues thereafter.

The second element of the vector stores the last timestep on which the timestep was reset to a new value. The scalar and vector values calculated by this fix are "intensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

- timestep

**Default:**

The option defaults is units = lattice.
**fix efield command**

**Syntax:**

```plaintext
fix ID group-ID efield ex ey ez
```

- `ID, group-ID` are documented in `fix` command
- `efield = style name of this fix command`
- `ex, ey, ez = E-field component values (electric field units)`
- `any of ex, ey, ez can be a variable (see below)`

**Examples:**

```plaintext
fix kick external-field efield 1.0 0.0 0.0
fix kick external-field efield 0.0 0.0 v_oscillate
```

**Description:**

Add a force \( F = qE \) to each charged atom in the group due to an external electric field being applied to the system.

Any of the 3 quantities defining the E-field components can be specified as an equal-style or atom-style variable, namely \( ex, ey, ez \). If the value is a variable, it should be specified as \( v\_name \), where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the E-field component.

Equal-style variables can specify formulas with various mathematical functions, and include `thermo_style` command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent E-field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent E-field with optional time-dependence as well.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the `fix_modify` options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various `output commands`. No parameter of this fix can be used with the `start/stop` keywords of the `run` command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

- `fix addforce`

**Default:** none
fix enforce2d command

fix enforce2d/cuda command

Syntax:

fix ID group-ID enforce2d

- ID, group-ID are documented in fix command
- enforce2d = style name of this fix command

Examples:

fix 5 all enforce2d

Description:

Zero out the z-dimension velocity and force on each atom in the group. This is useful when running a 2d simulation to insure that atoms do not move from their initial z coordinate.

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

Restrictions: none

Related commands: none

Default: none
fix evaporate command

Syntax:

fix ID group-ID evaporate N M region-ID seed

- ID, group-ID are documented in fix command
- evaporate = style name of this fix command
- N = delete atoms every this many timesteps
- M = number of atoms to delete each time
- region-ID = ID of region within which to perform deletions
- seed = random number seed to use for choosing atoms to delete
- zero or more keyword/value pairs may be appended

keyword = molecule
  molecule value = no or yes

Examples:

fix 1 solvent evaporate 1000 10 surface 49892
fix 1 solvent evaporate 1000 10 surface 38277 molecule yes

Description:

Remove M atoms from the simulation every N steps. This can be used, for example, to model evaporation of solvent particles or molecules (i.e. drying) of a system. Every N steps, the number of atoms in the fix group and within the specified region are counted. M of these are chosen at random and deleted. If there are less than M eligible particles, then all of them are deleted.

If the setting for the molecule keyword is no, then only single atoms are deleted. In this case, you should insure you do not delete only a portion of a molecule (only some of its atoms), or LAMMPS will soon generate an error when it tries to find those atoms. LAMMPS will warn you if any of the atoms eligible for deletion have a non-zero molecule ID, but does not check for this at the time of deletion.

If the setting for the molecule keyword is yes, then when an atom is chosen for deletion, the entire molecule it is part of is deleted. The count of deleted atoms is incremented by the number of atoms in the molecule, which may make it exceed M. If the molecule ID of the chosen atom is 0, then it is assumed to not be part of a molecule, and just the single atom is deleted.

As an example, if you wish to delete 10 water molecules every N steps, you should set M to 30. If only the water's oxygen atoms were in the fix group, then two hydrogen atoms would be deleted when an oxygen atom is selected for deletion, whether the hydrogens are inside the evaporation region or not.

Note that neighbor lists are re-built on timesteps that atoms are removed. Thus you should not remove atoms too frequently or you will incur overhead due to the cost of building neighbor lists.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.
This fix computes a global scalar, which can be accessed by various output commands. The scalar is the cumulative number of deleted atoms. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

fix deposit

**Default:**

The option defaults are molecule = no.
fix external command

Syntax:

fix ID group-ID external

- ID, group-ID are documented in fix command
- external = style name of this fix command

Examples:

fix 1 all external

Description:

This fix makes a callback each timestep or minimization iteration to an external driver program that is using LAMMPS as a library. This is a way to let another program compute forces on atoms which LAMMPS will include in its dynamics performed by the run command or its iterations performed by the minimize command.

The callback function "foo" will be invoked every timestep or iteration as:

foo(ptr,timestep,nlocal,ids,x,fexternal);

which has this prototype:

void foo(void *, int, int, int *, double **, double **);

The arguments are as follows:

- ptr = pointer provided by and simply passed back to external driver
- timestep = current LAMMPS timestep
- nlocal = # of atoms on this processor
- ids = list of atom IDs on this processor
- x = coordinates of atoms on this processor
- fexternal = forces on atoms on this processor

Fexternal are the forces returned by the driver program, which LAMMPS adds to the current force on each atom.

See the couple/lammps_quest/lmpqst.cpp file in the LAMMPS distribution for an example of a coupling application that uses this fix, and how it makes a call to the fix to specify what function the fix should callback to. The sample application performs classical MD using quantum forces computed by a density functional code Quest.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.
However, LAMMPS knows nothing about the energy associated with these forces. So you should perform the
minimization based on a force tolerance, not an energy tolerance.

**Restrictions:** none

**Related commands:** none

**Default:** none
fix freeze command

fix freeze/cuda command

Syntax:

fix ID group-ID freeze

- ID, group-ID are documented in fix command
- freeze = style name of this fix command

Examples:

fix 2 bottom freeze

Description:

Zero out the force and torque on a granular particle. This is useful for preventing certain particles from moving in a simulation. The granular pair styles also detect if this fix has been defined and compute interactions between frozen and non-frozen particles appropriately, as if the frozen particle has infinite mass.

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various output commands. This is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:
This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

There can only be a single freeze fix defined. This is because other the granular pair styles treat frozen particles differently and need to be able to reference a single group to which this fix is applied.

**Related commands:** none

atom_style sphere

**Default:** none
**fix gcmc command**

**Syntax:**

```plaintext
fix ID group-ID gcmc N X M type seed T mu displace keyword values ...
```

- ID, group-ID are documented in fix command
- gcmc = style name of this fix command
- N = invoke this fix every N steps
- X = number of exchanges to attempt every N steps
- M = number of MC displacements to attempt every N steps
- type = atom type of exchanged particles
- seed = random # seed (positive integer)
- T = temperature of the ideal gas reservoir (temperature units)
- mu = chemical potential of the ideal gas reservoir (energy units)
- displace = maximum Monte Carlo displacement distance (length units)
- zero or more keyword/value pairs may be appended to args
- keyword = molecule or region

  molecule value = no or yes
  region value = region-ID
  region-ID = ID of region to use as an exchange/move volume

**Examples:**

```plaintext
fix 2 all gcmc 10 1000 1000 1 29494 298.0 -0.5 0.01
fix 3 all gcmc 10 100 100 1 3456543 3.0 -2.5 0.1 molecule yes
fix 4 all gcmc 1 10 10 1 123456543 300.0 -12.5 1.0 region disk
```

**Description:**

This fix performs grand canonical Monte Carlo (GCMC) exchanges of particles of the given type with an imaginary ideal gas reservoir at the specified T and chemical potential (mu) as discussed in (Frenkel). If used with the fix nvt command, simulations in the grand canonical ensemble (muVT, constant chemical potential, constant volume, and constant temperature) can be performed. Specific uses include computing isotherms in microporous materials, or computing vapor-liquid coexistence curves.

Perform up to X exchanges of particles of the given type between the simulation domain and the imaginary reservoir every N timesteps. Also perform M Monte Carlo displacements of particles of the given type within the simulation domain. M should typically be chosen to be approximately equal to the expected number of particles of the given type within the domain, which will result in roughly one MC translation per particle per MC cycle.

This fix cannot be used to perform MC displacements of particles other than the exchanged type. All particles in the simulation domain can be moved using regular time integration displacements, e.g. via fix_nvt, resulting in a hybrid GCMC+MD simulation.

This command may optionally use the region keyword to define an exchange and move volume. The specified region must have been previously defined with a region command. It must be defined with side = in. Insertion attempts occur only within the specified region. Move and deletion attempt candidates are selected from particles within the region. If no candidate can be found within the specified region after randomly selecting candidates 1000 times, the move or deletion attempt is considered a failure. Moves must start within the specified region, but
may move the particle slightly outside of the region.

If used with fix_nvt, the temperature of the imaginary reservoir, T, should be set to be equivalent to the target
temperature used in fix_nvt. Otherwise, the imaginary reservoir will not be in thermal equilibrium with the
simulation domain.

Note that neighbor lists are re-built every timestep that this fix is invoked, so you should not set N to be too small.
However, periodic rebuilds are necessary in order to avoid dangerous rebuilds and missed interactions.
Specifically, avoid performing so many MC displacements per timestep that a particle can move beyond the
neighbor list skin distance. See the neighbor command for details.

When a particle is to be inserted, its coordinates are chosen as a random position within the current simulation
domain, and its velocity is randomly chosen from the specified temperature distribution given by T.

Exchanged particles have the specified atom type and are assigned to two groups: the default group "all" and the
group specified in the fix gcmc command (which can also be "all").

If the setting for the molecule keyword is no, then only single atoms are exchanged. In this case, you should
ensure you do not delete only a portion of a molecule (only some of its atoms), or LAMMPS will soon generate
an error when it tries to find those atoms. LAMMPS will warn you if any of the atoms eligible for deletion have a
non-zero molecule ID, but does not check for this at the time of deletion.

If the setting for the molecule keyword is yes, entire molecules are exchanged. This feature is not yet supported.

Use of this fix typically will cause the number of atoms to fluctuate, therefore, you will want to use the
compute_modify command to insure that the current number of atoms is used as a normalizing factor each time
temperature is computed. Here is the necessary command:

\[ \text{compute_modify thermo_temp dynamic yes} \]

If LJ units are used, note that a value of 0.18292026 is used by this fix as the reduced value for Planck's constant.
This value was derived from LJ parameters for argon, where \( h^* = h/\sqrt{\text{sigma}^2 \times \epsilon \times \text{mass}} \), \( \text{sigma} = 3.429 \) angstroms, \( \epsilon/k = 121.85 \) K, and \( \text{mass} = 39.948 \) amu.

\textbf{Restart, fix_modify, output, run start/stop, minimize info:}

This fix writes the state of the deposition to binary restart files. This includes information about the random
number generator seed, the next timestep for MC exchanges, etc. See the \texttt{read\_restart} command for info on how
to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an
uninterrupted fashion.

None of the fix\_modify options are relevant to this fix.

This fix computes a global vector of length 6, which can be accessed by various output commands. The vector
values are the following global cumulative quantities:

- 1 = displacement attempts
- 2 = displacement successes
- 3 = deletion attempts
- 4 = deletion successes
- 5 = insertion attempts
- 6 = insertion successes
The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Do not set "neigh_modify once yes" or else this fix will never be called. Reneighboring is required.

You cannot currently exchange charged particles or molecules with a net charge.

Only pairwise interactions, as defined by the pair_style command, are included in this calculation. Long-range interactions due to a kspace_style command are not included. Not all pair potentials can be evaluated in a pairwise mode as required by this fix. For example, 3-body potentials, such as Tersoff and Stillinger-Weber cannot be used. EAM potentials for metals only include the pair potential portion of the EAM interaction, not the embedding term.

**Related commands:**

fix_nvt, neighbor, fix_deposit, fix_evaporate

**Default:**

The option defaults are molecule = no.

fix gravity command

fix gravity/cuda command

fix gravity/omp command

Syntax:

fix ID group gravity style magnitude args

- ID, group are documented in fix command
- gravity = style name of this fix command
- magnitude = size of acceleration (force/mass units)
- magnitude can be a variable (see below)
- style = chute or spherical or gradient or vector

chute args = angle
    angle = angle in +x away from -z or -y axis in 3d/2d (in degrees)
    angle can be a variable (see below)

spherical args = phi theta
    phi = azimuthal angle from +x axis (in degrees)
    theta = angle from +z or +y axis in 3d/2d (in degrees)
    phi or theta can be a variable (see below)

vector args = x y z
    x y z = vector direction to apply the acceleration
    x or y or z can be a variable (see below)

Examples:

fix 1 all gravity 1.0 chute 24.0
fix 1 all gravity v_increase chute 24.0
fix 1 all gravity 1.0 spherical 0.0 -180.0
fix 1 all gravity 10.0 spherical v_phi v_theta
fix 1 all gravity 100.0 vector 1 1 0

Description:

Impose an additional acceleration on each particle in the group. This fix is typically used with granular systems to include a "gravity" term acting on the macroscopic particles. More generally, it can represent any kind of driving field, e.g. a pressure gradient inducing a Poiseuille flow in a fluid. Note that this fix operates differently than the fix addforce command. The addforce fix adds the same force to each atom, independent of its mass. This command imparts the same acceleration to each atom (force/mass).

The magnitude of the acceleration is specified in force/mass units. For granular systems (LJ units) this is typically 1.0. See the units command for details.

Style chute is typically used for simulations of chute flow where the specified angle is the chute angle, with flow occurring in the +x direction. For 3d systems, the tilt is away from the z axis; for 2d systems, the tilt is away from the y axis.

Style spherical allows an arbitrary 3d direction to be specified for the acceleration vector. Phi and theta are defined in the usual spherical coordinates. Thus for acceleration acting in the -z direction, theta would be 180.0
Theta = 90.0 and phi = -90.0 would mean acceleration acts in the -y direction. For 2d systems, phi is ignored and theta is an angle in the xy plane where theta = 0.0 is the y-axis.

Style vector imposes an acceleration in the vector direction given by (x,y,z). Only the direction of the vector is important; it's length is ignored. For 2d systems, the z component is ignored.

Any of the quantities magnitude, angle, phi, theta, x, y, z which define the gravitational magnitude and direction, can be specified as an equal-style variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the quantity. You should insure that the variable calculates a result in the appropriate units, e.g. force/mass or degrees.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent gravitational field.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify energy option is supported by this fix to add the gravitational potential energy of the system to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. This scalar is the gravitational potential energy of the particles in the defined field, namely mass * (g dot x) for each particles, where x and mass are the particles position and mass, and g is the gravitational field. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:
atom_style sphere, fix addforce

Default: none
fix heat command

Syntax:

fix ID group-ID heat N eflux

- ID, group-ID are documented in fix command
- heat = style name of this fix command
- N = add/subtract heat every this many timesteps
- eflux = rate of heat addition or subtraction (energy/time units)
- zero or more keyword/value pairs may be appended to args
- keyword = region

  region value = region-ID
  region-ID = ID of region atoms must be in to have added force

Examples:

fix 3 qin heat 1 1.0
fix 4 qout heat 1 -1.0 region top

Description:

Add non-translational kinetic energy (heat) to a group of atoms such that their aggregate momentum is conserved. Two of these fixes can be used to establish a temperature gradient across a simulation domain by adding heat (energy) to one group of atoms (hot reservoir) and subtracting heat from another (cold reservoir). E.g. a simulation sampling from the McDLT ensemble.

If the region keyword is used, the atom must be in both the group and the specified geometric region in order to have energy added or subtracted to it. If not specified, then the atoms in the group are affected wherever they may move to.

Heat addition/subtraction is performed every N timesteps. The eflux parameter determines the change in aggregate energy of the entire group of atoms per unit time, e.g. in eV/psec for metal units. Thus it is an "extensive" quantity, meaning its magnitude should be scaled with the number of atoms in the group. Since eflux is independent of N or the timestep, a larger value of N will add/subtract a larger amount of energy each time the fix is invoked. If heat is subtracted from the system too aggressively so that the group's kinetic energy would go to zero, LAMMPS halts with an error message.

Fix heat is different from a thermostat such as fix nvt or fix temp/rescale in that energy is added/subtracted continually. Thus if there isn't another mechanism in place to counterbalance this effect, the entire system will heat or cool continuously. You can use multiple heat fixes so that the net energy change is 0.0 or use fix viscous to drain energy from the system.

This fix does not change the coordinates of its atoms; it only scales their velocities. Thus you must still use an integration fix (e.g. fix nve) on the affected atoms. This fix should not normally be used on atoms that have their temperature controlled by another fix - e.g. fix nvt or fix langevin fix.

Restart, fix_modify, output, run start/stop, minimize info:
No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. This scalar is the most recent value by which velocities were scaled. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

compute temp, compute temp/region

**Default:** none
fix imd command

Syntax:

fix ID group-ID imd trate port keyword values ... 

• ID, group-ID are documented in fix command 
• imd = style name of this fix command 
• port = port number on which the fix listens for an IMD client 
• keyword = unwrap or fscale or trate

unwrap arg = on or off 
    off = coordinates are wrapped back into the principal unit cell (default) 
    on = "unwrapped" coordinates using the image flags used 

fscale arg = factor 
    factor = floating point number to scale IMD forces (default: 1.0) 

trate arg = transmission rate of coordinate data sets (default: 1) 

nowait arg = on or off 
    off = LAMMPS waits to be connected to an IMD client before continuing (default) 
    on = LAMMPS listens for an IMD client, but continues with the run

Examples:

fix vmd all imd 5678 
fix comm all imd 8888 trate 5 unwrap on fscale 10.0

Description:

This fix implements the "Interactive MD" (IMD) protocol which allows realtime visualization and manipulation of MD simulations through the IMD protocol, as initially implemented in VMD and NAMD. Specifically it allows LAMMPS to connect an IMD client, for example the VMD visualization program, so that it can monitor the progress of the simulation and interactively apply forces to selected atoms.

If LAMMPS is compiled with the preprocessor flag -DLAMMPS_ASYNC_IMD then fix imd will use POSIX threads to spawn a IMD communication thread on MPI rank 0 in order to offload data reading and writing from the main execution thread and potentially lower the inferred latencies for slow communication links. This feature has only been tested under linux.

There are example scripts for using this package with LAMMPS in examples/USER/imd. Additional examples and a driver for use with the Novint Falcon game controller as haptic device can be found at: http://sites.google.com/site/akohlmey/software/vrpn-icms.

The source code for this fix includes code developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign. We thank them for providing a software interface that allows codes like LAMMPS to hook to VMD.

Upon initialization of the fix, it will open a communication port on the node with MPI task 0 and wait for an incoming connection. As soon as an IMD client is connected, the simulation will continue and the fix will send the current coordinates of the fix's group to the IMD client at every trate MD step. When using r-RESPA, trate applies to the steps of the outmost RESPA level. During a run with an active IMD connection also the IMD client can request to apply forces to selected atoms of the fix group.
The port number selected must be an available network port number. On many machines, port numbers < 1024 are reserved for accounts with system manager privilege and specific applications. If multiple imd fixes would be active at the same time, each needs to use a different port number.

The nowait keyword controls the behavior of the fix when no IMD client is connected. With the default setting of off, LAMMPS will wait until a connection is made before continuing with the execution. Setting nowait to on will have the LAMMPS code be ready to connect to a client, but continue with the simulation. This can for example be used to monitor the progress of an ongoing calculation without the need to be permanently connected or having to download a trajectory file.

The trate keyword allows to select how often the coordinate data is sent to the IMD client. It can also be changed on request of the IMD client through an IMD protocol message. The unwrap keyword allows to send "unwrapped" coordinates to the IMD client that undo the wrapping back of coordinates into the principle unit cell, as done by default in LAMMPS. The fscale keyword allows to apply a scaling factor to forces transmitted by the IMD client. The IMD protocols stipulates that forces are transferred in kcal/mol/angstrom under the assumption that coordinates are given in angstrom. For LAMMPS runs with different units or as a measure to tweak the forces generated by the manipulation of the IMD client, this option allows to make adjustments.

To connect VMD to a listening LAMMPS simulation on the same machine with fix imd enabled, one needs to start VMD and load a coordinate or topology file that matches the fix group. When the VMD command prompts appears, one types the command line:

```
imd connect localhost 5678
```

This assumes that fix imd was started with 5678 as a port number for the IMD protocol.

The steps to do interactive manipulation of a running simulation in VMD are the following:

In the Mouse menu of the VMD Main window, select "Mouse -> Force -> Atom". You may alternately select "Residue", or "Fragment" to apply forces to whole residues or fragments. Your mouse can now be used to apply forces to your simulation. Click on an atom, residue, or fragment and drag to apply a force. Click quickly without moving the mouse to turn the force off. You can also use a variety of 3D position trackers to apply forces to your simulation. Game controllers or haptic devices with force-feedback such as the Novint Falcon or Sensable PHANTOM allow you to feel the resistance due to inertia or interactions with neighbors that the atoms experience you are trying to move, as if they were real objects. See the VMD IMD Homepage and the VRPN-ICMS Homepage for more details.

If IMD control messages are received, a line of text describing the message and its effect will be printed to the LAMMPS output screen, if screen output is active.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global scalar or vector or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.
When used in combination with VMD, a topology or coordinate file has to be loaded, which matches (in number and ordering of atoms) the group the fix is applied to. The fix internally sorts atom IDs by ascending integer value; in VMD (and thus the IMD protocol) those will be assigned 0-based consecutive index numbers.

When using multiple active IMD connections at the same time, each needs to use a different port number.

**Related commands:** none

**Default:** none
fix indent command

Syntax:

fix ID group-ID indent K keyword values ...

- ID, group-ID are documented in fix command
- indent = style name of this fix command
- K = force constant for indenter surface (force/distance^2 units)
- one or more keyword/value pairs may be appended
- keyword = sphere or cylinder or plane or side or units

sphere args = x y z R
  x,y,z = initial position of center of indenter (distance units)
  R = sphere radius of indenter (distance units)
  any of x,y,z,R can be a variable (see below)
cylinder args = dim c1 c2 R
  dim = x or y or z = axis of cylinder
  c1,c2 = coords of cylinder axis in other 2 dimensions (distance units)
  R = cylinder radius of indenter (distance units)
  any of c1,c2,R can be a variable (see below)
plane args = dim pos side
  dim = x or y or z = plane perpendicular to this dimension
  pos = position of plane in dimension x, y, or z (distance units)
  pos can be a variable (see below)
  side = lo or hi
side value = in or out
  in = the indenter acts on particles inside the sphere or cylinder
  out = the indenter acts on particles outside the sphere or cylinder
units value = lattice or box
  lattice = the geometry is defined in lattice units
  box = the geometry is defined in simulation box units

Examples:

fix 1 all indent 10.0 sphere 0.0 0.0 15.0 3.0
fix 1 all indent 10.0 sphere v_x v_y 0.0 v_radius side in
fix 2 flow indent 10.0 cylinder z 0.0 0.0 10.0 units box

Description:

Insert an indenter within a simulation box. The indenter repels all atoms that touch it, so it can be used to push into a material or as an obstacle in a flow. Or it can be used as a constraining wall around a simulation; see the discussion of the side keyword below.

The indenter can either be spherical or cylindrical or planar. You must set one of those 3 keywords.

A spherical indenter exerts a force of magnitude

\[ F(r) = -K (r - R)^2 \]

on each atom where \( K \) is the specified force constant, \( r \) is the distance from the atom to the center of the indenter, and \( R \) is the radius of the indenter. The force is repulsive and \( F(r) = 0 \) for \( r > R \).
A cylindrical indenter exerts the same force, except that \( r \) is the distance from the atom to the center axis of the cylinder. The cylinder extends infinitely along its axis.

Spherical and cylindrical indenters account for periodic boundaries in two ways. First, the center point of a spherical indenter \((x,y,z)\) or axis of a cylindrical indenter \((c_1,c_2)\) is remapped back into the simulation box, if the box is periodic in a particular dimension. This occurs every timestep if the indenter geometry is specified with a variable (see below), e.g. it is moving over time. Second, the calculation of distance to the indenter center or axis accounts for periodic boundaries. Both of these mean that an indenter can effectively move through and straddle one or more periodic boundaries.

A planar indenter is really an axis-aligned infinite-extent wall exerting the same force on atoms in the system, where \( R \) is the position of the plane and \( r-R \) is the distance from the plane. If the \textit{side} parameter of the plane is specified as \textit{lo} then it will indent from the \textit{lo} end of the simulation box, meaning that atoms with a coordinate less than the plane's current position will be pushed towards the \textit{hi} end of the box and atoms with a coordinate higher than the plane's current position will feel no force. Vice versa if \textit{side} is specified as \textit{hi}.

Any of the 4 quantities defining a spherical indenter's geometry can be specified as an equal-style variable, namely \( x, y, z, \) or \( R \). Similarly, for a cylindrical indenter, any of \( c_1, c_2, \) or \( R \), can be a variable. For a planar indenter, \( pos \) can be a variable. If the value is a variable, it should be specified as \texttt{v_name}, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to define the indenter geometry.

Note that equal-style variables can specify formulas with various mathematical functions, and include \texttt{thermo_style} command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify indenter properties that change as a function of time or span consecutive runs in a continuous fashion. For the latter, see the \texttt{start} and \texttt{stop} keywords of the \texttt{run} command and the \texttt{elaplong} keyword of \texttt{thermo_style custom} for details.

For example, if a spherical indenter's \( x \)-position is specified as \texttt{v_x}, then this variable definition will keep it's center at a relative position in the simulation box, \( 1/4 \) of the way from the left edge to the right edge, even if the box size changes:

\[
\text{variable x equal } "xlo + 0.25*lx"
\]

Similarly, either of these variable definitions will move the indenter from an initial position at 2.5 at a constant velocity of 5:

\[
\text{variable x equal } "2.5 + 5*elaplong*dt"
\text{variable x equal vdisplace(2.5,5)}
\]

If a spherical indenter's radius is specified as \texttt{v_r}, then these variable definitions will grow the size of the indenter at a specified rate.

\[
\text{variable r0 equal 0.0}
\text{variable rate equal 1.0}
\text{variable r equal } "v_r0 + step*dt*v_rate"
\]

If the \texttt{side} keyword is specified as \textit{out}, which is the default, then particles outside the indenter are pushed away from its outer surface, as described above. This only applies to spherical or cylindrical indenters. If the \texttt{side} keyword is specified as \textit{in}, the action of the indenter is reversed. Particles inside the indenter are pushed away from its inner surface. In other words, the indenter is now a containing wall that traps the particles inside it. If the radius shrinks over time, it will squeeze the particles.
The *units* keyword determines the meaning of the distance units used to define the indenter geometry. A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacing. The (x,y,z) coords of the indenter position are scaled by the x,y,z lattice spacings respectively. The radius of a spherical or cylindrical indenter is scaled by the x lattice spacing.

Note that the units keyword only affects indenter geometry parameters specified directly with numbers, not those specified as variables. In the latter case, you should use the *xlat*, *ylat*, *zlat* keywords of the *thermo_style* command if you want to include lattice spacings in a variable formula.

The force constant $K$ is not affected by the *units* keyword. It is always in force/distance$^2$ units where force and distance are defined by the *units* command. If you wish $K$ to be scaled by the lattice spacing, you can define $K$ with a variable whose formula contains *xlat*, *ylat*, *zlat* keywords of the *thermo_style* command, e.g.

```plaintext
variable k equal 100.0/xlat/xlat
fix 1 all indent $k sphere ...
```

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files.

The *fix_modify energy* option is supported by this fix to add the energy of interaction between atoms and the indenter to the system's potential energy as part of thermodynamic output. The energy of each particle interacting with the indenter is $K/3 (r - R)^3$.

This fix computes a global scalar energy and a global 3-vector of forces (on the indenter), which can be accessed by various *output commands*. The scalar and vector values calculated by this fix are "extensive".

The forces due to this fix are imposed during an energy minimization, invoked by the *minimize* command. Note that if you define the indenter geometry with a variable using a time-dependent formula, LAMMPS uses the iteration count in the minimizer as the timestep. But it is almost certainly a bad idea to have the indenter change its position or size during a minimization. LAMMPS does not check if you have done this.

**IMPORTANT NOTE:** If you want the atom/indenter interaction energy to be included in the total potential energy of the system (the quantity being minimized), you must enable the *fix_modify energy* option for this fix.

**Restrictions:** none

**Related commands:** none

**Default:**

The option defaults are side = out and units = lattice.
fix langevin command

Syntax:

fix ID group-ID langevin Tstart Tstop damp seed keyword values ...

- ID, group-ID are documented in fix command
- langevin = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
  - Tstart can be a variable (see below)
- damp = damping parameter (time units)
- seed = random number seed to use for white noise (positive integer)
- zero or more keyword/value pairs may be appended
- keyword = angmom or omega or scale or tally or zero

angmom value = no or yes
  - no = do not thermostat rotational degrees of freedom via the angular momentum
  - yes = do thermostat rotational degrees of freedom via the angular momentum

omega value = no or yes
  - no = do not thermostat rotational degrees of freedom via the angular velocity
  - yes = do thermostat rotational degrees of freedom via the angular velocity

scale values = type ratio
  - type = atom type (1-N)
  - ratio = factor by which to scale the damping coefficient

tally value = no or yes
  - no = do not tally the energy added/subtracted to atoms
  - yes = do tally the energy added/subtracted to atoms

zero value = no or yes
  - no = do not set total random force to zero
  - yes = set total random force to zero

Examples:

fix 3 boundary langevin 1.0 1.0 1000.0 699483
fix 1 all langevin 1.0 1.1 100.0 48279 scale 3 1.5

Description:

Apply a Langevin thermostat as described in (Schneider) to a group of atoms which models an interaction with a background implicit solvent. Used with fix nve, this command performs Brownian dynamics (BD), since the total force on each atom will have the form:

\[ F = F_c + F_f + F_r \]

\[ F_f = -\frac{m}{damp} v \]

\[ F_r \text{ is proportional to } \sqrt{K_B T m / (dt \text{ damp})} \]

\[ F_c \text{ is the conservative force computed via the usual inter-particle interactions (pair_style, bond_style, etc).} \]

The Ff and Fr terms are added by this fix on a per-particle basis. See the pair_style dpd/tstat command for a thermostating option that adds similar terms on a pairwise basis to pairs of interacting particles.

Ff is a frictional drag or viscous damping term proportional to the particle's velocity. The proportionality constant for each atom is computed as \( m/damp \), where \( m \) is the mass of the particle and damp is the damping factor.
Fr is a force due to solvent atoms at a temperature T randomly bumping into the particle. As derived from the fluctuation/dissipation theorem, its magnitude as shown above is proportional to $\sqrt{K_b T m / dt \text{ damp}}$, where $K_b$ is the Boltzmann constant, $T$ is the desired temperature, $m$ is the mass of the particle, $dt$ is the timestep size, and damp is the damping factor. Random numbers are used to randomize the direction and magnitude of this force as described in (Dunweg), where a uniform random number is used (instead of a Gaussian random number) for speed.

Note that unless you use the omega or angmom keywords, the thermostat effect of this fix is applied to only the translational degrees of freedom for the particles, which is an important consideration if extended spherical or aspherical particles, which have rotational degrees of freedom, are being thermostatted. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

IMPORTANT NOTE: Unlike the fix nvt command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies forces to effect thermostatting. Thus you must use a separate time integration fix, like fix nve to actually update the velocities and positions of atoms using the modified forces. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by fix nvt or fix temp/rescale commands.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

The desired temperature at each timestep is a ramped value during the run from $T_{\text{start}}$ to $T_{\text{stop}}$.

$T_{\text{start}}$ can be specified as an equal-style or atom-style variable. In this case, the $T_{\text{stop}}$ setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent temperature with optional time-dependence as well.

Like other fixes that perform thermostatting, this fix can be used with compute commands that remove a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or removing the x-component of velocity from the calculation. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

The damp parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the units command). The damp factor can be thought of as inversely related to the viscosity of the solvent. I.e. a small relaxation time implies a hi-viscosity solvent and vice versa. See the discussion about gamma and viscosity in the documentation for the fix viscous command for more details.
The random #seed must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The keyword/value option pairs are used in the following ways.

The keyword angmom and omega keywords enable thermostating of rotational degrees of freedom in addition to the usual translational degrees of freedom. This can only be done for finite-size particles. A simulation using atom_style sphere defines an omega for finite-size spheres. A simulation using atom_style ellipsoid defines a finite size and shape for aspherical particles and an angular momentum. The Langevin formulas for thermostating the rotational degrees of freedom are the same as those above, where force is replaced by torque, m is replaced by the moment of inertia I, and v is replaced by omega (which is derived from the angular momentum in the case of aspherical particles). The rotational temperature of the particles can be monitored by the compute temp/sphere and compute temp/asphere commands with their rotate options.

The keyword scale allows the damp factor to be scaled up or down by the specified factor for atoms of that type. This can be useful when different atom types have different sizes or masses. It can be used multiple times to adjust damp for several atom types. Note that specifying a ratio of 2 increases the relaxation time which is equivalent to the solvent's viscosity acting on particles with 1/2 the diameter. This is the opposite effect of scale factors used by the fix viscous command, since the damp factor in fix langevin is inversely related to the gamma factor in fix viscous. Also note that the damping factor in fix langevin includes the particle mass in Ff, unlike fix viscous. Thus the mass and size of different atom types should be accounted for in the choice of ratio values.

The keyword tally enables the calculation of the cumulative energy added/subtracted to the atoms as they are thermostatted. Effectively it is the energy exchanged between the infinite thermal reservoir and the particles. As described below, this energy can then be printed out or added to the potential energy of the system to monitor energy conservation.

The keyword zero can be used to eliminate drift due to the thermostat. Because the random forces on different atoms are independent, they do not sum exactly to zero. As a result, this fix applies a small random force to the entire system, and the center-of-mass of the system undergoes a slow random walk. If the keyword zero is set to yes, the total random force is set exactly to zero by subtracting off an equal part of it from each atom in the group. As a result, the center-of-mass of a system with zero initial momentum will not drift over time.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

The fix_modify temp option is supported by this fix. You can use it to assign a temperature compute you have defined to this fix which will be used in its thermostating procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The fix_modify energy option is supported by this fix to add the energy change induced by Langevin thermostating to the system's potential energy as part of thermodynamic output. Note that use of this option requires setting the tally keyword to yes.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive". Note that calculation of this quantity requires setting the tally keyword to yes.
This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the *run* command. See the *run* command for details of how to do this.

This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

fix nvt, fix temp/rescale, fix viscous, fix nvt, pair_style dpd/tstat

**Default:**

The option defaults are angmom = no, omega = no, scale = 1.0 for all types, tally = no, zero = no.

---


(Schneider) Schneider and Stoll, Phys Rev B, 17, 1302 (1978).
fix langevin/eff command

Syntax:

fix ID group-ID langevin/eff Tstart Tstop damp seed keyword values ...

- ID, group-ID are documented in fix command
- langevin/eff = style name of this fix command
- Tstart, Tstop = desired temperature at start/end of run (temperature units)
- damp = damping parameter (time units)
- seed = random number seed to use for white noise (positive integer)
- zero or more keyword/value pairs may be appended

keyword = scale or tally or zero
  scale values = type ratio
    type = atom type (1-N)
    ratio = factor by which to scale the damping coefficient
  tally values = no or yes
    no = do not tally the energy added/subtracted to atoms
    yes = do tally the energy added/subtracted to atoms

  zero value = no or yes
    no = do not set total random force to zero
    yes = set total random force to zero

Examples:

fix 3 boundary langevin/eff 1.0 1.0 10.0 699483
fix 1 all langevin/eff 1.0 1.1 10.0 48279 scale 3 1.5

Description:

Apply a Langevin thermostat as described in (Schneider) to a group of nuclei and electrons in the electron force field model. Used with fix nve/eff, this command performs Brownian dynamics (BD), since the total force on each atom will have the form:

\[ F = F_c + F_f + F_r \]

\[ F_f = - \frac{m}{damp} \cdot v \]

\[ F_r \text{ is proportional to } sqrt(K_b T m / (dt \cdot damp)) \]

\( F_c \) is the conservative force computed via the usual inter-particle interactions (pair_style).

The \( F_f \) and \( F_r \) terms are added by this fix on a per-particle basis.

The operation of this fix is exactly like that described by the fix langevin command, except that the thermostatting is also applied to the radial electron velocity for electron particles.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.
The `fix_modify temp` option is supported by this fix. You can use it to assign a temperature `compute` you have defined to this fix which will be used in its thermostating procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The `fix_modify energy` option is supported by this fix to add the energy change induced by Langevin thermostating to the system's potential energy as part of thermodynamic output. Note that use of this option requires setting the `tally` keyword to `yes`.

This fix computes a global scalar which can be accessed by various `output commands`. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive". Note that calculation of this quantity requires setting the `tally` keyword to `yes`.

This fix can ramp its target temperature over multiple runs, using the `start` and `stop` keywords of the `run` command. See the `run` command for details of how to do this.

This fix is not invoked during energy minimization.

**Restrictions:** none

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the *Making LAMMPS* section for more info.

**Related commands:**

`fix langevin`

**Default:**

The option defaults are scale = 1.0 for all types and tally = no.

---


(Schneider) Schneider and Stoll, Phys Rev B, 17, 1302 (1978).
fix lineforce command

Syntax:

fix ID group-ID lineforce x y z

- ID, group-ID are documented in fix command
- lineforce = style name of this fix command
- x y z = direction of line as a 3-vector

Examples:

fix hold boundary lineforce 0.0 1.0 1.0

Description:

Adjust the forces on each atom in the group so that only the component of force along the linear direction specified by the vector (x,y,z) remains. This is done by subtracting out components of force in the plane perpendicular to the line.

If the initial velocity of the atom is 0.0 (or along the line), then it should continue to move along the line thereafter.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

Restrictions: none

Related commands:

fix planeforce

Default: none
fix meso command

Syntax:

fix ID group-ID meso

• ID, group-ID are documented in fix command
• meso = style name of this fix command

Examples:

fix 1 all meso

Description:

Perform time integration to update position, velocity, internal energy and local density for atoms in the group each timestep. This fix is needed to time-integrate mesoscopic systems where particles carry internal variables such as SPH or DPDE.

See this PDF guide to using SPH in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

"fix meso/stationary"

Default: none
**fix meso/stationary command**

**Syntax:**

```plaintext
fix ID group-ID meso/stationary
```

- ID, group-ID are documented in fix command
- meso = style name of this fix command

**Examples:**

```plaintext
fix 1 boundary meso/stationary
```

**Description:**

Perform time integration to update internal energy and local density, but not position or velocity for atoms in the group each timestep. This fix is needed for SPH simulations to correctly time-integrate fixed boundary particles which constrain a fluid to a given region in space.

See this PDF guide to using SPH in LAMMPS.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

"fix meso"

**Default:** none
**fix_modify command**

**Syntax:**

```
fix_modify fix-ID keyword value ...
```

- `fix-ID` = ID of the fix to modify
- one or more keyword/value pairs may be appended
- `keyword` = `temp` or `press` or `energy`

  - `temp` value = compute ID that calculates a temperature
  - `press` value = compute ID that calculates a pressure
  - `energy` value = yes or no

**Examples:**

```
fix_modify 3 temp myTemp press myPress
fix_modify 1 energy yes
```

**Description:**

Modify one or more parameters of a previously defined fix. Only specific fix styles support specific parameters. See the doc pages for individual fix commands for info on which ones support which fix_modify parameters.

The `temp` keyword is used to determine how a fix computes temperature. The specified compute ID must have been previously defined by the user via the `compute` command and it must be a style of compute that calculates a temperature. All fixes that compute temperatures define their own compute by default, as described in their documentation. Thus this option allows the user to override the default method for computing T.

The `press` keyword is used to determine how a fix computes pressure. The specified compute ID must have been previously defined by the user via the `compute` command and it must be a style of compute that calculates a pressure. All fixes that compute pressures define their own compute by default, as described in their documentation. Thus this option allows the user to override the default method for computing P.

For fixes that calculate a contribution to the potential energy of the system, the `energy` keyword will include that contribution in thermodynamic output of potential energy. See the `thermo_style` command for info on how potential energy is output. The contribution by itself can be printed by using the keyword f_ID in the thermo_style custom command, where ID is the fix-ID of the appropriate fix. Note that you must use this setting for a fix if you are using it when performing an energy minimization and if you want the energy and forces it produces to be part of the optimization criteria.

**Restrictions:** none

**Related commands:**

- `fix`, `compute temp`, `compute pressure`, `thermo_style`

**Default:**

The option defaults are temp = ID defined by fix, press = ID defined by fix, energy = no.
fix momentum command

Syntax:

fix ID group-ID momentum N keyword values ...

- ID, group-ID are documented in fix command
- momentum = style name of this fix command
- N = adjust the momentum every this many timesteps one or more keyword/value pairs may be appended
- keyword = linear or angular

linear values = xflag yflag zflag
  xflag, yflag, zflag = 0/1 to exclude/include each dimension
angular values = none

Examples:

fix 1 all momentum 1 linear 1 1 0
fix 1 all momentum 100 linear 1 1 1 angular

Description:

Zero the linear and/or angular momentum of the group of atoms every N timesteps by adjusting the velocities of the atoms. One (or both) of the linear or angular keywords must be specified.

If the linear keyword is used, the linear momentum is zeroed by subtracting the center-of-mass velocity of the group from each atom. This does not change the relative velocity of any pair of atoms. One or more dimensions can be excluded from this operation by setting the corresponding flag to 0.

If the angular keyword is used, the angular momentum is zeroed by subtracting a rotational component from each atom.

This command can be used to insure the entire collection of atoms (or a subset of them) does not drift or rotate during the simulation due to random perturbations (e.g. fix langevin thermostatting).

Note that the velocity command can be used to create initial velocities with zero aggregate linear and/or angular momentum.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix recenter, velocity
Default: none
fix move command

Syntax:

fix ID group-ID move style args keyword values ...

- ID, group-ID are documented in fix command
- move = style name of this fix command
- style = linear or wiggle or rotate or variable

linear args = Vx Vy Vz
  Vx,Vy,Vz = components of velocity vector (velocity units), any component can be specified as NULL

wiggle args = Ax Ay Az period
  Ax,Ay,Az = components of amplitude vector (distance units), any component can be specified as NULL
  period = period of oscillation (time units)

rotate args = Px Py Pz Rx Ry Rz period
  Px,Py,Pz = origin point of axis of rotation (distance units)
  Rx,Ry,Rz = axis of rotation vector
  period = period of rotation (time units)

variable args = v_dx v_dy v_dz v_vx v_vy v_vz
  v_dx,v_dy,v_dz = 3 variable names that calculate x,y,z displacement as function of time, any component can be specified as NULL
  v_vx,v_vy,v_vz = 3 variable names that calculate x,y,z velocity as function of time, any component can be specified as NULL

- zero or more keyword/value pairs may be appended
- keyword = units

units value = box or lattice

Examples:

fix 1 boundary move wiggle 3.0 0.0 0.0 1.0 units box
fix 2 boundary move rotate 0.0 0.0 0.0 0.0 0.0 1.0 5.0
fix 2 boundary move variable v_myx v_myy NULL v_VX v_VY NULL

Description:

Perform updates of position and velocity for atoms in the group each timestep using the specified settings or formulas, without regard to forces on the atoms. This can be useful for boundary or other atoms, whose movement can influence nearby atoms.

IMPORTANT NOTE: The atoms affected by this fix should not normally be time integrated by other fixes (e.g. fix nve, fix nvt), since that will change their positions and velocities twice.

IMPORTANT NOTE: As atoms move due to this fix, they will pass thru periodic boundaries and be remapped to the other side of the simulation box, just as they would during normal time integration (e.g. via the fix nve command). It is up to you to decide whether periodic boundaries are appropriate with the kind of atom motion you are prescribing with this fix.

IMPORTANT NOTE: As discussed below, atoms are moved relative to their initial position at the time the fix is specified. These initial coordinates are stored by the fix in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this fix by using the set image command.
The linear style moves atoms at a constant velocity, so that their position \( X = (x,y,z) \) as a function of time is given in vector notation as

\[
X(t) = X_0 + V \times \delta \tag{1}
\]

where \( X_0 = (x_0,y_0,z_0) \) is their position at the time the fix is specified, \( V \) is the specified velocity vector with components \( (V_x,V_y,V_z) \), and \( \delta \) is the time elapsed since the fix was specified. This style also sets the velocity of each atom to \( V = (V_x,V_y,V_z) \). If any of the velocity components is specified as NULL, then the position and velocity of that component is time integrated the same as the fix nve command would perform, using the corresponding force component on the atom.

Note that the linear style is identical to using the variable style with an equal-style variable that uses the vdisplace() function. E.g.

```plaintext
variable V equal 10.0
variable x equal vdisplace(0.0,$V)
fix 1 boundary move variable v_x NULL NULL v_V NULL NULL
```

The wiggle style moves atoms in an oscillatory fashion, so that their position \( X = (x,y,z) \) as a function of time is given in vector notation as

\[
X(t) = X_0 + A \sin(\omega \times \delta) \tag{2}
\]

where \( X_0 = (x_0,y_0,z_0) \) is their position at the time the fix is specified, \( A \) is the specified amplitude vector with components \( (A_x,A_y,A_z) \), \( \omega \) is \( 2 \pi / \text{period} \), and \( \delta \) is the time elapsed since the fix was specified. This style also sets the velocity of each atom to the time derivative of this expression. If any of the amplitude components is specified as NULL, then the position and velocity of that component is time integrated the same as the fix nve command would perform, using the corresponding force component on the atom.

Note that the wiggle style is identical to using the variable style with equal-style variables that use the swiggle() and cwiggle() functions. E.g.

```plaintext
variable A equal 10.0
variable T equal 5.0
variable omega equal 2.0*PI/$T
variable x equal swiggle(0.0,$A,$T)
variable v equal v_omega*($A-cwiggle(0.0,$A,$T))
fix 1 boundary move variable v_x NULL NULL v_V NULL NULL
```

The rotate style rotates atoms around a rotation axis \( R = (R_x,R_y,R_z) \) that goes thru a point \( P = (P_x,P_y,P_z) \). The period of the rotation is also specified. This style also sets the velocity of each atom to \( (\omega \times \text{Rperp}) \) where \( \omega \) is its angular velocity around the rotation axis and \( \text{Rperp} \) is a perpendicular vector from the rotation axis to the atom. If the defined atom_style assigns an angular velocity to each atom, then each atom's angular velocity is also set to \( \omega \). Note that the direction of rotation for the atoms around the rotation axis is consistent with the right-hand rule: if your right-hand's thumb points along \( R \), then your fingers wrap around the axis in the direction of rotation.

The variable style allows the position and velocity components of each atom to be set by formulas specified via the variable command. Each of the 6 variables is specified as an argument to the fix as v_name, where name is the variable name that is defined elsewhere in the input script.

Each variable must be of either the equal or atom style. Equal-style variables compute a single numeric quantity, that can be a function of the timestep as well as of other simulation values. Atom-style variables compute a numeric quantity for each atom, that can be a function per-atom quantities, such as the atom's position, as well as...
of the timestep and other simulation values. Note that this fix stores the original coordinates of each atom (see note below) so that per-atom quantity can be used in an atom-style variable formula. See the `variable` command for details.

The first 3 variables \((v_{dx}, v_{dy}, v_{dz})\) specified for the `variable` style are used to calculate a displacement from the atom's original position at the time the fix was specified. The second 3 variables \((v_{vx}, v_{vy}, v_{vz})\) specified are used to compute a velocity for each atom.

Any of the 6 variables can be specified as NULL. If both the displacement and velocity variables for a particular \(x,y,z\) component are specified as NULL, then the position and velocity of that component is time integrated the same as the `fix nve` command would perform, using the corresponding force component on the atom. If only the velocity variable for a component is specified as NULL, then the displacement variable will be used to set the position of the atom, and its velocity component will not be changed. If only the displacement variable for a component is specified as NULL, then the velocity variable will be used to set the velocity of the atom, and the position of the atom will be time integrated using that velocity.

The `units` keyword determines the meaning of the distance units used to define the linear velocity and wiggle amplitude and rotate origin. This setting is ignored for the `variable` style. A `box` value selects standard units as defined by the `units` command, e.g. velocity in Angstroms/fmsec and amplitude and position in Angstroms for units = real. A `lattice` value means the velocity units are in lattice spacings per time and the amplitude and position are in lattice spacings. The `lattice` command must have been previously used to define the lattice spacing. Each of these 3 quantities may be dependent on the \(x,y,z\) dimension, since the lattice spacings can be different in \(x,y,z\).

For rRESPA time integration, this fix adjusts the position and velocity of atoms on the outermost rRESPA level.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the original coordinates of moving atoms to binary restart files, so that the motion can be continuous in a restarted simulation. See the `read_restart` command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the `fix_modify` options are relevant to this fix.

This fix produces a per-atom array which can be accessed by various output commands. The number of columns for each atom is 3, and the columns store the original unwrapped \(x,y,z\) coords of each atom. The per-atom values can be accessed on any timestep.

No parameter of this fix can be used with the `start/stop` keywords of the `run` command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

- `fix nve`

**Default:** none

The option default is units = lattice.
**fix msst command**

**Syntax:**

```plaintext
fix ID group-ID msst dir shockvel keyword value ...
```

- **ID, group-ID** are documented in **fix** command
- **msst** = style name of this fix
- **dir** = x or y or z
- **shockvel** = shock velocity (strictly positive, distance/time units)
- **zero or more keyword value pairs may be appended**
- **keyword** = q or mu or p0 or v0 or e0 or tscale

```plaintext
q value = cell mass-like parameter (mass^2/distance^4 units)
mu value = artificial viscosity (mass/length/time units)
p0 value = initial pressure in the shock equations (pressure units)
v0 value = initial simulation cell volume in the shock equations (distance^3 units)
e0 value = initial total energy (energy units)
tscale value = reduction in initial temperature (unitless fraction between 0.0 and 1.0)
```

**Examples:**

```plaintext
fix 1 all msst y 100.0 q 1.0e5 mu 1.0e5
fix 2 all msst z 50.0 q 1.0e4 mu 1.0e4 v0 4.3419e+03 p0 3.7797e+03 e0 -9.72360e+02 tscale 0.01
```

**Description:**

This command performs the Multi-Scale Shock Technique (MSST) integration to update positions and velocities each timestep to mimic a compressive shock wave passing over the system. See [Reed](#) for a detailed description of this method. The MSST varies the cell volume and temperature in such a way as to restrain the system to the shock Hugoniot and the Rayleigh line. These restraints correspond to the macroscopic conservation laws dictated by a shock front. **shockvel** determines the steady shock velocity that will be simulated.

To perform a simulation, choose a value of **q** that provides volume compression on the timescale of 100 fs to 1 ps. If the volume is not compressing, either the shock speed is chosen to be below the material sound speed or **p0** has been chosen inaccurately. Volume compression at the start can be sped up by using a non-zero value of **tscale**. Use the smallest value of **tscale** that results in compression.

Under some special high-symmetry conditions, the pressure (volume) and/or temperature of the system may oscillate for many cycles even with an appropriate choice of mass-like parameter **q**. Such oscillations have physical significance in some cases. The optional **mu** keyword adds an artificial viscosity that helps break the system symmetry to equilibrate to the shock Hugoniot and Rayleigh line more rapidly in such cases.

**tscale** is a factor between 0 and 1 that determines what fraction of thermal kinetic energy is converted to compressive strain kinetic energy at the start of the simulation. Setting this parameter to a non-zero value may assist in compression at the start of simulations where it is slow to occur.

If keywords **e0**, **p0**, or **v0** are not supplied, these quantities will be calculated on the first step, after the energy specified by **tscale** is removed. The value of **e0** is not used in the dynamical equations, but is used in calculating the deviation from the Hugoniot.
Values of shockvel less than a critical value determined by the material response will not have compressive solutions. This will be reflected in lack of significant change of the volume in the MSST.

For all pressure styles, the simulation box stays orthogonal in shape. Parrinello-Rahman boundary conditions (tilted box) are supported by LAMMPS, but are not implemented for MSST.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp" and "pressure", as if these commands had been issued:

```plaintext
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp
```

See the compute temp and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press". The group for the new computes is "all".

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the state of all internal variables to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The progress of the MSST can be monitored by printing the global scalar and global vector quantities computed by the fix.

The scalar is the cumulative energy change due to the fix. This is also the energy added to the potential energy by the fix_modify energy command. With this command, the thermo keyword etotal prints the conserved quantity of the MSST dynamic equations. This can be used to test if the MD timestep is sufficiently small for accurate integration of the dynamic equations. See also thermo_style command.

The global vector contains four values in this order:

```
[dhugoniot, drayleigh, lagrangian_speed, lagrangian_position]
```

1. dhugoniot is the departure from the Hugoniot (temperature units).
2. drayleigh is the departure from the Rayleigh line (pressure units).
3. lagrangian_speed is the laboratory-frame Lagrangian speed (particle velocity) of the computational cell (velocity units).
4. lagrangian_position is the computational cell position in the reference frame moving at the shock speed. This is usually a good estimate of distance of the computational cell behind the shock front.

To print these quantities to the log file with descriptive column headers, the following LAMMPS commands are suggested:

```plaintext
fix          msst all msst z
fix_modify   msst energy yes
variable dhug equal f_msst[1]
variable dray equal f_msst[2]
variable lgr_vel equal f_msst[3]
variable lgr_pos equal f_msst[4]
thermo_style custom step temp ke pe lz pzz etotal v_dhug v_dray v_lgr_vel v_lgr_pos f_msst
```

These fixes compute a global scalar and a global vector of 4 quantities, which can be accessed by various output commands. The scalar values calculated by this fix are "extensive"; the vector values are "intensive".
Restrictions:

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

All cell dimensions must be periodic. This fix can not be used with a triclinic cell. The MSST fix has been tested only for the group-ID all.

Related commands:

fix nphug, fix deform

Default:

The keyword defaults are q = 10, mu = 0, tscale = 0.01. p0, v0, and e0 are calculated on the first step.

**fix neb command**

**Syntax:**

```
fix ID group-ID neb Kspring
```

- ID, group-ID are documented in fix command
- neb = style name of this fix command
- Kspring = inter-replica spring constant (force/distance units)

**Examples:**

```
fix 1 active neb 10.0
```

**Description:**

Add inter-replica forces to atoms in the group for a multi-replica simulation run via the *neb* command to perform a nudged elastic band (NEB) calculation for transition state finding. Hi-level explanations of NEB are given with the *neb* command and in Section **howto** 5 of the manual. The fix neb command must be used with the "neb" command to define how inter-replica forces are computed.

Only the N atoms in the fix group experience inter-replica forces. Atoms in the two end-point replicas do not experience these forces, but those in intermediate replicas do. During the initial stage of NEB, the 3N-length vector of interatomic forces $F_i = -\text{Grad}(V)$ acting on the atoms of each intermediate replica I is altered, as described in the *(Henkelman1)* paper, to become:

$$F_i = -\text{Grad}(V) + (\text{Grad}(V) \cdot \text{That}) \text{That} + K_{spring} (|R_{i+1} - R_i| - |R_i - R_{i-1}|) \text{That}$$

$R_i$ are the atomic coordinates of replica I; $R_{i-1}$ and $R_{i+1}$ are the coordinates of its neighbor replicas. That ($\hat{t}$ with a hat over it) is the unit "tangent" vector for replica I which is a function of $R_i$, $R_{i-1}$, $R_{i+1}$, and the potential energy of the 3 replicas; it points roughly in the direction of $(R_{i+1} - R_{i-1})$; see the *(Henkelman1)* paper for details.

The first two terms in the above equation are the component of the interatomic forces perpendicular to the tangent vector. The last term is a spring force between replica I and its neighbors, parallel to the tangent vector direction with the specified spring constant $K_{spring}$.

The effect of the first two terms is to push the atoms of each replica toward the minimum energy path (MEP) of conformational states that transition over the energy barrier. The MEP for an energy barrier is defined as a sequence of 3N-dimensional states which cross the barrier at its saddle point, each of which has a potential energy gradient parallel to the MEP itself.

The effect of the last term is to push each replica away from its two neighbors in a direction along the MEP, so that the final set of states are equidistant from each other.

During the second stage of NEB, the forces on the N atoms in the replica nearest the top of the energy barrier are altered so that it climbs to the top of the barrier and finds the saddle point. The forces on atoms in this replica are described in the *(Henkelman2)* paper, and become:

$$F_i = -\text{Grad}(V) + 2 (\text{Grad}(V) \cdot \text{That}) \text{That}$$

The inter-replica forces for the other replicas are unchanged from the first equation.
Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, as invoked by the minimize command via the neb command.

Restrictions:

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

Related commands:

neb

Default: none


fix nvt command

fix nvt/cuda command

fix npt command

fix npt/cuda command

fix nph command

Syntax:

fix ID group-ID style_name keyword value ... 

• ID, group-ID are documented in fix command 
• style_name = nvt or npt or nph 

one or more keyword value pairs may be appended

keyword = temp or iso or aniso or tri or x or y or z or xy or yz or xz or couple or tchain or pchain or mtk or tloop or ploop or nreset or drag or dilate or scalexy or scaleyz or scalexz or flip or fixedpoint 

• temp values = Tstart Tstop Tdamp
  Tstart, Tstop = external temperature at start/end of run
  Tdamp = temperature damping parameter (time units)
• iso or aniso or tri values = Pstart Pstop Pdamp
  Pstart, Pstop = scalar external pressure at start/end of run (pressure units)
  Pdamp = pressure damping parameter (time units)
• x or y or z or xy or yz or xz values = Pstart Pstop Pdamp
  Pstart, Pstop = external stress tensor component at start/end of run (pressure units)
  Pdamp = stress damping parameter (time units)
• couple = none or xyz or xy or yz or xz
• tchain value = N
  N = length of thermostat chain (1 = single thermostat)
• pchain values = N
  N length of thermostat chain on barostat (0 = no thermostat)
• mtk value = yes or no
  = add in MTK adjustment term or not
• tloop value = M
  M = number of sub-cycles to perform on thermostat
• ploop value = M
  M = number of sub-cycles to perform on barostat thermostat
• nreset value = reset reference cell every this many timesteps
• drag value = Df
  Df = drag factor added to barostat/thermostat (0.0 = no drag)
• dilate value = dilate-group-ID
  dilate-group-ID = only dilate atoms in this group due to barostat volume changes
• scalexy value = yes or no
  = scale xy with ly
• scaleyz value = yes or no
  = scale yz with lz
• scalexz value = yes or no
  = scale xz with lz
• flip value = yes or no
  = allow or disallow box flips when it becomes highly skewed
• fixedpoint values = x y z
  x, y, z = perform barostat dilation/contraction around this point (distance units)

Examples:

fix 1 all nvt temp 300.0 300.0 100.0
fix 1 water npt temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 jello npt temp 300.0 300.0 100.0 tri 5.0 5.0 1000.0
fix 2 ice nph x 1.0 1.0 0.5 y 2.0 2.0 0.5 z 3.0 3.0 0.5 yz 0.1 0.1 0.5 xz 0.2 0.2 0.5 xy 0.3 0.3 0.5
Description:

These commands perform time integration on Nose-Hoover style non-Hamiltonian equations of motion which are
designed to generate positions and velocities sampled from the canonical (nvt), isothermal-isobaric (npt), and
isenthalpic (nph) ensembles. This updates the position and velocity for atoms in the group each timestep.

The thermostating and barostatting is achieved by adding some dynamic variables which are coupled to the
particle velocities (thermostatting) and simulation domain dimensions (barostatting). In addition to basic
thermostatting and barostatting, these fixes can also create a chain of thermostats coupled to the particle
thermostat, and another chain of thermostats coupled to the barostat variables. The barostat can be coupled to the
overall box volume, or to individual dimensions, including the $xy$, $xz$ and $yz$ tilt dimensions. The external pressure
of the barostat can be specified as either a scalar pressure (isobaric ensemble) or as components of a symmetric
stress tensor (constant stress ensemble). When used correctly, the time-averaged temperature and stress tensor of
the particles will match the target values specified by $T_{\text{start}}$/$T_{\text{stop}}$ and $P_{\text{start}}$/$P_{\text{stop}}$.

The equations of motion used are those of Shinoda et al in (Shinoda), which combine the hydrostatic equations of
Martyna, Tobias and Klein in (Martyna) with the strain energy proposed by Parrinello and Rahman in
(Parrinello). The time integration schemes closely follow the time-reversible measure-preserving Verlet and
rRESPA integrators derived by Tuckerman et al. in (Tuckerman).

The thermostat parameters for fix styles nvt and npt is specified using the temp keyword. Other thermostat-related
keywords are tchain, tloop and drag, which are discussed below.

The thermostat is applied to only the translational degrees of freedom for the particles. The translational degrees
of freedom can also have a bias velocity removed before thermostatting takes place; see the description below.
The desired temperature at each timestep is a ramped value during the run from $T_{\text{start}}$ to $T_{\text{stop}}$. The $T_{\text{damp}}$
parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value
of 10.0 means to relax the temperature in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the
units command). The atoms in the fix group are the only ones whose velocities and positions are updated by the
velocity/position update portion of the integration.

IMPORTANT NOTE: A Nose-Hoover thermostat will not work well for arbitrary values of $T_{\text{damp}}$. If $T_{\text{damp}}$ is
too small, the temperature can fluctuate wildly; if it is too large, the temperature will take a very long time to
equilibrate. A good choice for many models is a $T_{\text{damp}}$ of around 100 timesteps. Note that this is NOT the same
as 100 time units for most units settings.

The barostat parameters for fix styles npt and nph is specified using one or more of the iso, aniso, tri, x, y, z, xy,
xz, yz, and couple keywords. These keywords give you the ability to specify all 6 components of an external stress
tensor, and to couple various of these components together so that the dimensions they represent are varied
together during a constant-pressure simulation.

Other barostat-related keywords are pchain, mtk, ploop, nreset, drag, and dilate, which are discussed below.

Orthogonal simulation boxes have 3 adjustable dimensions (x,y,z). Triclinic (non-orthogonal) simulation boxes
have 6 adjustable dimensions (x,y,z,xy,xz,yz). The create_box, read data, and read_restart commands specify
whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the $xy$,xz,yz tilt
factors.

The target pressures for each of the 6 components of the stress tensor can be specified independently via the $x$, $y$,
$z$, $xy$, $xz$, $yz$ keywords, which correspond to the 6 simulation box dimensions. For each component, the external
pressure or tensor component at each timestep is a ramped value during the run from $P_{\text{start}}$ to $P_{\text{stop}}$. If a target
pressure is specified for a component, then the corresponding box dimension will change during a simulation. For
example, if the \textit{y} keyword is used, the \textit{y}-box length will change. If the \textit{xy} keyword is used, the \textit{xy} tilt factor will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the \texttt{fix deform} command.

Note that in order to use the \textit{xy}, \textit{xz}, or \textit{yz} keywords, the simulation box must be triclinic, even if its initial tilt factors are 0.0.

For all barostat keywords, the \textit{Pdamp} parameter operates like the \textit{Tdamp} parameter, determining the time scale on which pressure is relaxed. For example, a value of 10.0 means to relax the pressure in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the \texttt{units} command).

\textbf{IMPORTANT NOTE:} A Nose-Hoover barostat will not work well for arbitrary values of \textit{Pdamp}. If \textit{Pdamp} is too small, the pressure and volume can fluctuate wildly; if it is too large, the pressure will take a very long time to equilibrate. A good choice for many models is a \textit{Pdamp} of around 1000 timesteps. Note that this is NOT the same as 1000 time units for most \texttt{units} settings.

Regardless of what atoms are in the \texttt{fix} group (the only atoms which are time integrated), a global pressure or stress tensor is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword \texttt{dilate} is specified with a \texttt{dilate-group-ID} for a group that represents a subset of the atoms. This can be useful, for example, to leave the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid. This option should be used with care, since it can be unphysical to dilate some atoms and not others, because it can introduce large, instantaneous displacements between a pair of atoms (one dilated, one not) that are far from the dilation origin. Also note that for atoms not in the \texttt{fix} group, a separate time integration fix like \texttt{fix nve} or \texttt{fix nvt} can be used on them, independent of whether they are dilated or not.

The \texttt{couple} keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, \texttt{xz} means the \textit{Pxx} and \textit{Pzz} components of the stress tensor are coupled. \texttt{Xyz} means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The \textit{Pstart}, \textit{Pstop}, \textit{Pdamp} parameters for any coupled dimensions must be identical. \texttt{Couple xyz} can be used for a 2d simulation; the \textit{z} dimension is simply ignored.

The \texttt{iso}, \texttt{aniso}, and \texttt{tri} keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword \texttt{iso} means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "\texttt{iso }\texttt{Pstart }\texttt{Pstop }\texttt{Pdamp}" is the same as specifying these 4 keywords:

\begin{verbatim}
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple xyz
\end{verbatim}

The keyword \texttt{aniso} means \texttt{x}, \texttt{y}, and \texttt{z} dimensions are controlled independently using the \textit{Pxx}, \textit{Pyy}, and \textit{Pzz} components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "\texttt{aniso }\texttt{Pstart }\texttt{Pstop }\texttt{Pdamp}" is the same as specifying these 4 keywords:

\begin{verbatim}
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
\end{verbatim}
The keyword *tri* means \( x, y, z, xy, xz, \) and \( yz \) dimensions are controlled independently using their individual stress components as the driving forces, and the specified scalar pressure as the external normal stress. Using "tri Pstart Pstop Pdamp" is the same as specifying these 7 keywords:

\[
\begin{align*}
x & \quad \text{Pstart} \quad \text{Pstop} \quad \text{Pdamp} \\
y & \quad \text{Pstart} \quad \text{Pstop} \quad \text{Pdamp} \\
z & \quad \text{Pstart} \quad \text{Pstop} \quad \text{Pdamp} \\
xy & \quad 0.0 \quad 0.0 \quad \text{Pdamp} \\
yz & \quad 0.0 \quad 0.0 \quad \text{Pdamp} \\
xz & \quad 0.0 \quad 0.0 \quad \text{Pdamp} \\
couple & \quad \text{none}
\end{align*}
\]

In some cases (e.g. for solids) the pressure (volume) and/or temperature of the system can oscillate undesirably when a Nose/Hoover barostat and thermostat is applied. The optional *drag* keyword will damp these oscillations, although it alters the Nose/Hoover equations. A value of 0.0 (no drag) leaves the Nose/Hoover formalism unchanged. A non-zero value adds a drag term; the larger the value specified, the greater the damping effect. Performing a short run and monitoring the pressure and temperature is the best way to determine if the drag term is working. Typically a value between 0.2 to 2.0 is sufficient to damp oscillations after a few periods. Note that use of the drag keyword will interfere with energy conservation and will also change the distribution of positions and velocities so that they do not correspond to the nominal NVT, NPT, or NPH ensembles.

An alternative way to control initial oscillations is to use chain thermostats. The keyword *tchain* determines the number of thermostats in the particle thermostat. A value of 1 corresponds to the original Nose-Hoover thermostat. The keyword *pchain* specifies the number of thermostats in the chain thermostatting the barostat degrees of freedom. A value of 0 corresponds to no thermostatting of the barostat variables.

The *mtk* keyword controls whether or not the correction terms due to Martyna, Tuckerman, and Klein are included in the equations of motion (Martyna). Specifying *no* reproduces the original Hoover barostat, whose volume probability distribution function differs from the true NPT and NPH ensembles by a factor of \( 1/V \). Hence using *yes* is more correct, but in many cases the difference is negligible.

The keyword *tloop* can be used to improve the accuracy of integration scheme at little extra cost. The initial and final updates of the thermostat variables are broken up into *tloop* substeps, each of length \( dt/tloop \). This corresponds to using a first-order Suzuki-Yoshida scheme (Tuckerman2006). The keyword *ploop* does the same thing for the barostat thermostat.

The keyword *nreset* controls how often the reference dimensions used to define the strain energy are reset. If this keyword is not used, or is given a value of zero, then the reference dimensions are set to those of the initial simulation domain and are never changed. If the simulation domain changes significantly during the simulation, then the final average pressure tensor will differ significantly from the specified values of the external stress tensor. A value of *nstep* means that every *nstep* timesteps, the reference dimensions are set to those of the current simulation domain.

The *scaleyz*, *scalexz*, and *scalexy* keywords control whether or not the corresponding tilt factors are scaled with the associated box dimensions when barostatting triclinic periodic cells. The default values *yes* will turn on scaling, which corresponds to adjusting the linear dimensions of the cell while preserving its shape. Choosing *no* ensures that the tilt factors are not scaled with the box dimensions. See below for restrictions and default values in different situations. In older versions of LAMMPS, scaling of tilt factors was not performed. The old behavior can be recovered by setting all three scale keywords to *no*.
The *flip* keyword allows the tilt factors for a triclinic box to exceed half the distance of the parallel box length, as discussed below. If the *flip* value is set to *yes*, the bound is enforced by flipping the box when it is exceeded. If the *flip* value is set to *no*, the tilt will continue to change without flipping. Note that if applied stress induces large deformations (e.g. in a liquid), this means the box shape can tilt dramatically and LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

The *fixedpoint* keyword specifies the fixed point for barostat volume changes. By default, it is the center of the box. Whatever point is chosen will not move during the simulation. For example, if the lower periodic boundaries pass through (0,0,0), and this point is provided to *fixedpoint*, then the lower periodic boundaries will remain at (0,0,0), while the upper periodic boundaries will move twice as far. In all cases, the particle trajectories are unaffected by the chosen value, except for a time-dependent constant translation of positions.

**IMPORTANT NOTE:** Using a barostat coupled to tilt dimensions *xy*, *xz*, *yz* can sometimes result in arbitrarily large values of the tilt dimensions, i.e. a dramatically deformed simulation box. LAMMPS allows the tilt factors to grow a small amount beyond the normal limit of half the box length (0.6 times the box length), and then performs a box “flip” to an equivalent periodic cell. See the discussion of the *flip* keyword above, to allow this bound to be exceeded, if desired.

The flip operation is described in more detail in the doc page for *fix deform*. Both the barostat dynamics and the atom trajectories are unaffected by this operation. However, if a tilt factor is incremented by a large amount (1.5 times the box length) on a single timestep, LAMMPS can not accommodate this event and will terminate the simulation with an error. This error typically indicates that there is something badly wrong with how the simulation was constructed, such as specifying values of $P_{\text{start}}$ that are too far from the current stress value, or specifying a timestep that is too large. Triclinic barostatting should be used with care. This also is true for other barostat styles, although they tend to be more forgiving of insults. In particular, it is important to recognize that equilibrium liquids can not support a shear stress and that equilibrium solids can not support shear stresses that exceed the yield stress.

One exception to this rule is if the 1st dimension in the tilt factor (*x* for *xy*) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient due to the highly skewed simulation box.

**IMPORTANT NOTE:** Unlike the *fix temp/berendsen* command which performs thermostatting but NO time integration, these fixes perform thermostatting/barostatting AND time integration. Thus you should not use any other time integration fix, such as *fix nve* on atoms to which this fix is applied. Likewise, the *temp* options for *fix nvt* and *fix npt* should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by *fix langevin* or *fix temp/rescale* commands.

See **this howto section** of the manual for a discussion of different ways to compute temperature and perform thermostatting and barostatting.

These fixes compute a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp" and "pressure", as if one of these two sets of commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp
```

```compute fix-ID_temp all temp
compute fix-ID_press all pressure fix-ID_temp
```
See the `compute temp` and `compute pressure` commands for details. Note that the IDs of the new computes are the `fix-ID + underscore + "temp"` or `fix_ID + underscore + "press"`. For fix nvt, the group for the new computes is the same as the fix group. For fix nph and fix npt, the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the `thermo_style` command) with ID = `thermo_temp` and `thermo_press`. This means you can change the attributes of this fix's temperature or pressure via the `compute_modify` command or print this temperature or pressure during thermodynamic output via the `thermo_style custom` command using the appropriate compute-ID. It also means that changing attributes of `thermo_temp` or `thermo_press` will have no effect on this fix.

Like other fixes that perform thermostatting, fix nvt and fix npt can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the `fix_modify` command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

These fixes can be used with either the `verlet` or `respa` integrators. When using one of the barostat fixes with `respa`, LAMMPS uses an integrator constructed according to the following factorization of the Liouville propagator (for two rRESPA levels):

\[
\exp \left( iL \Delta t \right) = \exp \left( iL_{T\text{-baro}} \frac{\Delta t}{2} \right) \exp \left( iL_{T\text{-part}} \frac{\Delta t}{2} \right) \exp \left( iL_{\epsilon,2} \frac{\Delta t}{2} \right) \exp \left( iL_{2}^{(2)} \frac{\Delta t}{2} \right) \\
\times \left[ \exp \left( iL_{2}^{(1)} \frac{\Delta t}{2n} \right) \exp \left( iL_{\epsilon,1} \frac{\Delta t}{n} \right) \exp \left( iL_{1} \frac{\Delta t}{n} \right) \exp \left( iL_{2}^{(1)} \frac{\Delta t}{2n} \right) \right]^{n} \\
\times \exp \left( iL_{2}^{(2)} \frac{\Delta t}{2} \right) \exp \left( iL_{\epsilon,2} \frac{\Delta t}{2} \right) \exp \left( iL_{T\text{-part}} \frac{\Delta t}{2} \right) \exp \left( iL_{T\text{-baro}} \frac{\Delta t}{2} \right) \\
+ \mathcal{O} \left( \Delta t^{3} \right)
\]

This factorization differs somewhat from that of Tuckerman et al., in that the barostat is only updated at the outermost rRESPA level, whereas Tuckerman’s factorization requires splitting the pressure into pieces corresponding to the forces computed at each rRESPA level. In theory, the latter method will exhibit better numerical stability. In practice, because Pdamp is normally chosen to be a large multiple of the outermost rRESPA timestep, the barostat dynamics are not the limiting factor for numerical stability. Both factorizations are time-reversible and can be shown to preserve the phase space measure of the underlying non-Hamiltonian equations of motion.

Styles with a `cuda` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.
These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restart, fix_modify, output, run start/stop, minimize info:**

These fixes writes the state of all the thermostat and barostat variables to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify temp and press options are supported by these fixes. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure, as described above. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

IMPORTANT NOTE: If both the temp and press keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a pressure compute defines its own temperature compute as an argument when it is specified. The temp keyword will override this (for the pressure compute being used by fix npt), but only if the temp keyword comes after the press keyword. If the temp keyword comes before the press keyword, then the new pressure compute specified by the press keyword will be unaffected by the temp setting.

The fix_modify energy option is supported by these fixes to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of thermodynamic output.

These fixes compute a global scalar and a global vector of quantities, which can be accessed by various output commands. The scalar value calculated by these fixes is "extensive"; the vector values are "intensive".

The scalar is the cumulative energy change due to the fix.

The vector stores internal Nose/Hoover thermostat and barostat variables. The number and meaning of the vector values depends on which fix is used and the settings for keywords tchain and pchain, which specify the number of Nose/Hoover chains for the thermostat and barostat. If no thermostatting is done, then tchain is 0. If no barostatting is done, then pchain is 0. In the following list, "ndof" is 0, 1, 3, or 6, and is the number of degrees of freedom in the barostat. Its value is 0 if no barostat is used, else its value is 6 if any off-diagonal stress tensor component is barostatted, else its value is 1 if couple xyz is used or couple xy for a 2d simulation, otherwise its value is 3.

The order of values in the global vector and their meaning is as follows. The notation means there are tchain values for eta, followed by tchain for eta_dot, followed by ndof for omega, etc:

- eta[tchain] = particle thermostat displacements (unitless)
- eta_dot[tchain] = particle thermostat velocities (1/time units)
- omega[ndof] = barostat displacements (unitless)
- omega_dot[ndof] = barostat velocities (1/time units)
- etap[pchain] = barostat thermostat displacements (unitless)
etap_dot[pchain] = barostat thermostat velocities (1/time units)
PE_eta[tchain] = potential energy of each particle thermostat displacement (energy units)
KE_eta_dot[tchain] = kinetic energy of each particle thermostat velocity (energy units)
PE_omega[ndof] = potential energy of each barostat displacement (energy units)
KE_omega_dot[ndof] = kinetic energy of each barostat velocity (energy units)
PE_etap[pchain] = potential energy of each barostat thermostat displacement (energy units)
KE_etap_dot[pchain] = kinetic energy of each barostat thermostat velocity (energy units)
PE_strain[1] = scalar strain energy (energy units)

These fixes can ramp their external temperature and pressure over multiple runs, using the start and stop keywords of the run command. See the run command for details of how to do this.

These fixes are not invoked during energy minimization.

Restrictions:

X, y, z cannot be barostatted if the associated dimension is not periodic. Xy, xz, and yz can only be barostatted if the simulation domain is triclinic and the 2nd dimension in the keyword (y dimension in xy) is periodic. Z, xz, and yz, cannot be barostatted for 2D simulations. The create_box, read data, and read_restart commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

For the temp keyword, the final Tstop cannot be 0.0 since it would make the external T = 0.0 at some timestep during the simulation which is not allowed in the Nose/Hoover formulation.

The scaleyz yes and scalexz yes keyword/value pairs can not be used for 2D simulations. scaleyz yes, scalexz yes, and scalexy yes options can only be used if the 2nd dimension in the keyword is periodic, and if the tilt factor is not coupled to the barostat via keywords tri, yz, xz, and xy.

Related commands:

fix nve, fix_modify, run_style

Default:

The keyword defaults are tchain = 3, pchain = 3, mtk = yes, tloop = ploop = 1, nreset = 0, drag = 0.0, dilate = all, couple = none, scaleyz = scalexz = scalexy = yes if periodic in 2nd dimension and not coupled to barostat, otherwise no.


**fix nvt/eff command**

**fix npt/eff command**

**fix nph/eff command**

**Syntax:**

```
fix ID group-ID style_name keyword value ...
```

- ID, group-ID are documented in `fix` command
- `style_name = nvt/eff` or `npt/eff` or `nph/eff`

One or more keyword value pairs may be appended

`temp` or `iso` or `aniso` or `tri` or `x` or `y` or `z` or `xy` or `yz` or `xz` or couple or `tchain` or 

`Tstart,Tstop` = external temperature at start/end of run

`Tstart,Tstop` = temperature damping parameter (time units)

`iso` or `aniso` or `tri` values = `Pstart Pstop Pdamp`

`Pstart,Pstop` = scalar external pressure at start/end of run (pressure units)

`Pdamp` = pressure damping parameter (time units)

`x` or `y` or `z` or `xy` or `yz` or `xz` values = `Pstart Pstop Pdamp`

`Pstart,Pstop` = external stress tensor component at start/end of run (pressure units)

`Pdamp` = stress damping parameter (time units)

`couple` = none or `xyz` or `xy` or `yz` or `xz`

`tchain` value = length of thermostat chain (1 = single thermostat)

`pchain` values = length of thermostat chain on barostat (0 = no thermostat)

`mtk` value = yes or no = add in MTK adjustment term or not

`tloop` value = number of sub-cycles to perform on thermostat

`ploop` value = number of sub-cycles to perform on barostat thermostat

`nreset` value = reset reference cell every this many timesteps

`drag` value = drag factor added to barostat/thermostat (0.0 = no drag)

`dilate` value = all or partial

**Examples:**

```
fix 1 all nvt/eff temp 300.0 300.0 0.1
fix 1 part npt/eff temp 300.0 300.0 0.1 iso 0.0 0.0 1.0
fix 2 part npt/eff temp 300.0 300.0 0.1 tri 5.0 5.0 1.0
fix 2 ice nph/eff x 1.0 1.0 0.5 y 2.0 2.0 0.5 z 3.0 3.0 0.5 yz 0.1 0.1 0.5 zx 0.2 0.2 0.5 xy 0.3 0.3 0.5
```

**Description:**

These commands perform time integration on Nose-Hoover style non-Hamiltonian equations of motion for nuclei and electrons in the group for the electron force field model. The fixes are designed to generate positions and velocities sampled from the canonical (nvt), isothermal-isobaric (npt), and isenthalpic (nph) ensembles. This is achieved by adding some dynamic variables which are coupled to the particle velocities (thermostatting) and simulation domain dimensions (barostatting). In addition to basic thermostatting and barostatting, these fixes can also create a chain of thermostats coupled to the particle thermostat, and another chain of thermostats coupled to the barostat variables. The barostat can be coupled to the overall box volume, or to individual dimensions, including the `xy`, `xz` and `yz` tilt dimensions. The external pressure of the barostat can be specified as either a scalar pressure (isobaric ensemble) or as components of a symmetric stress tensor (constant stress ensemble). When used correctly, the time-averaged temperature and stress tensor of the particles will match the target values specified by `Tstart/Tstop` and `Pstart/Pstop`.
The operation of these fixes is exactly like that described by the fix nvt, npt, and nph commands, except that the radius and radial velocity of electrons are also updated. Likewise the temperature and pressure calculated by the fix, using the computes it creates (as discussed in the fix nvt, npt, and nph doc page), are performed with computes that include the eFF contribution to the temperature or kinetic energy from the electron radial velocity.

IMPORTANT NOTE: there are two different pressures that can be reported for eFF when defining the pair_style (see pair eff/cut to understand these settings), one (default) that considers electrons do not contribute radial virial components (i.e. electrons treated as incompressible 'rigid' spheres) and one that does. The radial electronic contributions to the virials are only tallied if the flexible pressure option is set, and this will affect both global and per-atom quantities. In principle, the true pressure of a system is somewhere in between the rigid and the flexible eFF pressures, but, for most cases, the difference between these two pressures will not be significant over long-term averaged runs (i.e. even though the energy partitioning changes, the total energy remains similar).

IMPORTANT NOTE: currently, there is no available option for the user to set or create temperature distributions that include the radial electronic degrees of freedom with the velocity command, so the the user must allow for these degrees of freedom to equilibrate (i.e. equi-partitioning of energy) through time integration.

**Restart, fix_modify, output, run start/stop, minimize info:**

See the doc page for the fix nvt, npt, and nph commands for details.

**Restrictions:**

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Other restriction discussed on the doc page for the fix nvt, npt, and nph commands also apply.

IMPORTANT NOTE: The temperature for systems (regions or groups) with only electrons and no nuclei is 0.0 (i.e. not defined) in the current temperature calculations, a practical example would be a uniform electron gas or a very hot plasma, where electrons remain delocalized from the nuclei. This is because, even though electron virials are included in the temperature calculation, these are averaged over the nuclear degrees of freedom only. In such cases a corrective term must be added to the pressure to get the correct kinetic contribution.

**Related commands:**

fix nvt, fix nph, fix npt, fix_modify, run_style

**Default:**

The keyword defaults are tchain = 3, pchain = 3, mtk = yes, tloop = ploop = 1, nreset = 0, drag = 0.0, dilate = all, and couple = none.

---


fix nph/asphere command

Syntax:

fix ID group-ID nph/asphere args keyword value ...

- ID, group-ID are documented in fix command
- nph/asphere = style name of this fix command
- additional barostat related keyword/value pairs from the fix nph command can be appended

Examples:

fix 1 all nph/asphere iso 0.0 0.0 1000.0
fix 2 all nph/asphere x 5.0 5.0 1000.0
fix 2 all nph/asphere x 5.0 5.0 1000.0 drag 0.2
fix 2 water nph/asphere aniso 0.0 0.0 1000.0 dilate partial

Description:

Perform constant NPH integration to update position, velocity, orientation, and angular velocity each timestep for aspherical or ellipsoidal particles in the group using a Nose/Hoover pressure barostat. P is pressure; H is enthalpy. This creates a system trajectory consistent with the isenthalpic ensemble.

This fix differs from the fix nph command, which assumes point particles and only updates their position and velocity.

Additional parameters affecting the barostat are specified by keywords and values documented with the fix nph command. See, for example, discussion of the aniso, and dilate keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPH integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword dilate is specified with a value of partial, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/asphere" and "pressure", as if these commands had been issued:

compute fix-ID_temp all temp/asphere
compute fix-ID_press all pressure fix-ID_temp

See the compute temp/asphere and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = thermo_temp and thermo_press. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the
thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of
thermo_temp or thermo_press will have no effect on this fix.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover barostat to binary restart files. See the read_restart command for info
on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an
uninterrupted fashion.

The fix_modify temp and press options are supported by this fix. You can use them to assign a compute you have
defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the
kinetic energy derived from the compute temperature should be consistent with the virial term computed using all
atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify energy option is supported by this fix to add the energy change induced by Nose/Hoover
barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nph command.

This fix can ramp its target pressure over multiple runs, using the start and stop keywords of the run command.
See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the
Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style
ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or
spherical as defined by their shape attribute.

Related commands:

fix nph, fix nve_asphere, fix nvt_asphere, fix npt_asphere, fix_modify

Default: none
fix nph/sphere command

Syntax:

fix ID group-ID nph/sphere args keyword value ...

• ID, group-ID are documented in fix command
• nph/sphere = style name of this fix command
• additional barostat related keyword/value pairs from the fix nph command can be appended

Examples:

fix 1 all nph/sphere iso 0.0 0.0 1000.0
fix 2 all nph/sphere x 5.0 5.0 1000.0
fix 2 all nph/sphere x 5.0 5.0 1000.0 drag 0.2
fix 2 water nph/sphere aniso 0.0 0.0 1000.0 dilate partial

Description:

Perform constant NPH integration to update position, velocity, and angular velocity each timestep for extended spherical particles in the group using a Nose/Hoover pressure barostat. P is pressure; H is enthalpy. This creates a system trajectory consistent with the isenthalpic ensemble.

This fix differs from the fix nph command, which assumes point particles and only updates their position and velocity.

Additional parameters affecting the barostat are specified by keywords and values documented with the fix nph command. See, for example, discussion of the aniso, and dilate keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPH integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword dilate is specified with a value of partial, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/sphere" and "pressure", as if these commands had been issued:

compute fix-ID_temp all temp/sphere
compute fix-ID_press all pressure fix-ID_temp

See the compute temp/sphere and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = thermo_temp and thermo_press. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the
thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of 
thermo_temp or thermo_press will have no effect on this fix.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the state of the Nose/Hoover barostat to binary restart files. See the read_restart command for info 
on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an 
uninterrupted fashion.

The fix_modify temp and press options are supported by this fix. You can use them to assign a compute you have 
defined to this fix which will be used in its thermostating or barostatting procedure. If you do this, note that the 
kinetic energy derived from the compute temperature should be consistent with the virial term computed using all 
atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify energy option is supported by this fix to add the energy change induced by Nose/Hoover 
barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nph command.

This fix can ramp its target pressure over multiple runs, using the start and stop keywords of the run command. 
See the run command for details of how to do this.

This fix is not invoked during energy minimization.

**Restrictions:**

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the atom_style 
sphere command.

All particles in the group must be finite-size spheres. They cannot be point particles.

**Related commands:**

fix nph, fix nve_sphere, fix nvt_sphere, fix npt_sphere, fix_modify

**Default:** none
**fix nphug command**

**Syntax:**

```
fix ID group-ID nphug keyword value ...
```

- **ID, group-ID** are documented in fix command
- one or more keyword value pairs may be appended
  - keyword = `temp` or `iso` or `aniso` or `tri` or `x` or `y` or `z` or `couple` or `tchain` or `pchain` or `mtk` or `tloop` or `ploop` or `nreset` or `drag` or `dilate` or `scaleyz` or `scalexz` or `scalexy`
  - temp values = `Valuel Value2 Tdamp`
    - `Valuel, Value2` = Nose-Hoover target temperatures, ignored by Hugoniostat
    - `Tdamp` = temperature damping parameter (time units)
  - `iso` or `aniso` or `tri` values = `Pstart Pstop Pdamp`
    - `Pstart, Pstop` = scalar external pressures, must be equal (pressure units)
    - `Pdamp` = pressure damping parameter (time units)
  - `x` or `y` or `z` or `xy` or `yz` or `xz` values = `Pstart Pstop Pdamp`
    - `Pstart, Pstop` = external stress tensor components, must be equal (pressure units)
    - `Pdamp` = stress damping parameter (time units)
  - `couple` = `none` or `xyz` or `xy` or `yz` or `xz`
  - `tchain` value = length of thermostat chain (1 = single thermostat)
  - `pchain` values = length of thermostat chain on barostat (0 = no thermostat)
  - `mtk` value = `yes` or `no` = add in MTK adjustment term or not
  - `tloop` value = number of sub-cycles to perform on thermostat
  - `ploop` value = number of sub-cycles to perform on barostat thermostat
  - `nreset` value = reset reference cell every this many timesteps
  - `drag` value = drag factor added to barostat/thermostat (0.0 = no drag)
  - `dilate` value = `all` or `partial`
  - `scaleyz` value = `yes` or `no` = scale yz with lz
  - `scalexz` value = `yes` or `no` = scale xz with lz
  - `scalexy` value = `yes` or `no` = scale xy with ly

**Examples:**

```
fix myhug all nphug temp 1.0 1.0 10.0 z 40.0 40.0 70.0
fix myhug all nphug temp 1.0 1.0 10.0 iso 40.0 40.0 70.0 drag 200.0 tchain 1 pchain 0
```

**Description:**

This command is a variant of the Nose-Hoover fix npt fix style. It performs time integration of the Hugoniostat equations of motion developed by Ravelo et al. (Ravelo). These equations compress the system to a state with average axial stress or pressure equal to the specified target value and that satisfies the Rankine-Hugoniot (RH) jump conditions for steady shocks.

The compression can be performed either hydrostatically (using keyword `iso, aniso, or tri`) or uniaxially (using keywords `x, y, or z`). In the hydrostatic case, the cell dimensions change dynamically so that the average axial stress in all three directions converges towards the specified target value. In the uniaxial case, the chosen cell dimension changes dynamically so that the average axial stress in that direction converges towards the target value. The other two cell dimensions are kept fixed (zero lateral strain).

This leads to the following additional restrictions on the keywords:

- One and only one of the following keywords should be used: `iso, aniso, tri, x, y, z`
- The specified initial and final target pressures must be the same.
- The keywords `xy, xz, yz` may not be used.
The only admissible value for the couple keyword is xyz, which has the same effect as keyword iso.

The temp keyword must be used to specify the time constant for kinetic energy relaxation, but initial and final target temperature values are ignored.

Essentially, a Hugoniostat simulation is an NPT simulation in which the user-specified target temperature is replaced with a time-dependent target temperature \( T_t \) obtained from the following equation:

\[
T_t - T = \frac{\left( \frac{1}{2} (P + P_0) (V_0 - V) + E_0 - E \right)}{N_{dof} k_B} = \Delta
\]

where \( T \) and \( T_t \) are the instantaneous and target temperatures, \( P \) and \( P_0 \) are the instantaneous and reference pressures or axial stresses, depending on whether hydrostatic or uniaxial compression is being performed, \( V \) and \( V_0 \) are the instantaneous and reference volumes, \( E \) and \( E_0 \) are the instantaneous and reference internal energy (potential plus kinetic), \( N_{dof} \) is the number of degrees of freedom used in the definition of temperature, and \( k_B \) is the Boltzmann constant. \( \Delta \) is the negative deviation of the instantaneous temperature from the target temperature. When the system reaches a stable equilibrium, the value of \( \Delta \) should fluctuate about zero.

The values of \( E_0, V_0, \) and \( P_0 \) are the instantaneous values at the start of the simulation. These can be overridden using the fix_modify keywords \( e0, v0, \) and \( p0 \) described below.

IMPORTANT NOTE: Unlike the fix temp/berendsen command which performs thermostatting but NO time integration, this fix performs thermostatting/barostatting AND time integration. Thus you should not use any other time integration fix, such as fix nve on atoms to which this fix is applied. Likewise, this fix should not be used on atoms that have their temperature controlled by another fix - e.g. by fix langevin or fix temp/rescale commands.

This fix computes a temperature and pressure at each timestep. To do this, the fix creates its own computes of style "temp" and "pressure", as if one of these two sets of commands had been issued:

```plaintext
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp
compute fix-ID_temp all temp
compute fix-ID_press all pressure fix-ID_temp
```

See the compute temp and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press". The group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = thermo_temp and thermo_press. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of thermo_temp or thermo_press will have no effect on this fix.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the values of \( E_0, V_0, \) and \( P_0 \), as well as the state of all the thermostat and barostat variables to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a
restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify e0, v0 and p0 keywords can be used to define the values of E0, V0, and P0. Note the the values for e0 and v0 are extensive, and so must correspond to the total energy and volume of the entire system, not energy and volume per atom. If any of these quantities are not specified, then the instantaneous value in the system at the start of the simulation is used.

The fix_modify temp and press options are supported by these fixes. You can use them to assign a compute you have defined to this fix which will be used in its thermostetting or barostetting procedure, as described above. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify energy option is supported by these fixes to add the energy change induced by Nose/Hoover thermostetting and barostetting to the system's potential energy as part of thermodynamic output. Either way, this energy is *not* included in the definition of internal energy E when calculating the value of Delta in the above equation.

These fixes compute a global scalar and a global vector of quantities, which can be accessed by various output commands. The scalar value calculated by these fixes is "extensive"; the vector values are "intensive".

The scalar is the cumulative energy change due to the fix.

The vector stores three quantities unique to this fix (Delta, Us, and up), followed by all the internal Nose/Hoover thermostat and barostat variables defined for fix_style npt. Delta is the deviation of the temperature from the target temperature, given by the above equation. Us and up are the shock and particle velocity corresponding to a steady shock calculated from the RH conditions. They have units of distance/time.

**Restrictions:**

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

All the usual restrictions for fix_style npt apply, plus the additional ones mentioned above.

**Related commands:**

fix msst, fix npt, fix_modify

**Default:**

The keyword defaults are the same as those for fix npt

**fix npt/asphere command**

**Syntax:**

```plaintext
fix ID group-ID npt/asphere keyword value ...
```

- ID, group-ID are documented in fix command
- npt/asphere = style name of this fix command
- additional thermostat and barostat related keyword/value pairs from the fix npt command can be appended

**Examples:**

```plaintext
fix 1 all npt/asphere temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 all npt/asphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0
fix 2 all npt/asphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0 drag 0.2
fix 2 water npt/asphere temp 300.0 300.0 100.0 aniso 0.0 0.0 1000.0 dilate partial
```

**Description:**

Perform constant NPT integration to update position, velocity, orientation, and angular velocity each timestep for aspherical or ellipsoidal particles in the group using a Nose/Hoover temperature thermostat and Nose/Hoover pressure barostat. P is pressure; T is temperature. This creates a system trajectory consistent with the isothermal-isobaric ensemble.

This fix differs from the fix npt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the aspherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat and barostat are specified by keywords and values documented with the fix npt command. See, for example, discussion of the `temp`, `iso`, `aniso`, and `dilate` keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPT integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword `dilate` is specified with a value of `partial`, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/asphere" and "pressure", as if these commands had been issued:

```plaintext
compute fix-ID_temp all temp/asphere
calculate fix-ID_press all pressure fix-ID_temp
```
See the compute temp/asphere and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = thermo_temp and thermo_press. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of thermo_temp or thermo_press will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the state of the Nose/Hoover thermostat and barostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify temp and press options are supported by this fix. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify energy option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix npt command.

This fix can ramp its target temperature and pressure over multiple runs, using the start and stop keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

**Related commands:**
fix npt, fix nve_asphere, fix nvt_asphere, fix_modify

Default: none
**fix npt/sphere command**

**Syntax:**

```plaintext
fix ID group-ID npt/sphere keyword value ...
```

- ID, group-ID are documented in fix command
- npt/sphere = style name of this fix command
- additional thermostat and barostat related keyword/value pairs from the fix npt command can be appended

**Examples:**

```plaintext
fix 1 all npt/sphere temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 all npt/sphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0
fix 2 all npt/sphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0 drag 0.2
fix 2 water npt/sphere temp 300.0 300.0 100.0 aniso 0.0 0.0 1000.0 dilate partial
```

**Description:**

Perform constant NPT integration to update position, velocity, and angular velocity each timestep for extended spherical particles in the group using a Nose/Hoover temperature thermostat and Nose/Hoover pressure barostat. P is pressure; T is temperature. This creates a system trajectory consistent with the isothermal-isobaric ensemble.

This fix differs from the fix npt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the spherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat and barostat are specified by keywords and values documented with the fix npt command. See, for example, discussion of the temp, iso, aniso, and dilate keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPT integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword dilate is specified with a value of partial, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/sphere" and "pressure", as if these commands had been issued:

```plaintext
compute fix-ID_temp all temp/sphere
compute fix-ID_press all pressure fix-ID_temp
```
See the `compute temp/sphere` and `compute pressure` commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the `thermo_style` command) with ID = `thermo_temp` and `thermo_press`. This means you can change the attributes of this fix's temperature or pressure via the `compute_modify` command or print this temperature or pressure during thermodynamic output via the `thermo_style custom` command using the appropriate compute-ID. It also means that changing attributes of `thermo_temp` or `thermo_press` will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with `compute commands` that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the `fix_modify` command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual `compute commands` to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the state of the Nose/Hoover thermostat and barostat to binary restart files. See the `read_restart` command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The `fix_modify temp` and `press` options are supported by this fix. You can use them to assign a `compute` you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The `fix_modify energy` option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the `fix npt` command.

This fix can ramp its target temperature and pressure over multiple runs, using the `start` and `stop` keywords of the `run` command. See the `run` command for details of how to do this.

This fix is not invoked during energy minimization.

**Restrictions:**

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the `atom_style sphere` command.

All particles in the group must be finite-size spheres. They cannot be point particles.

**Related commands:**

`fix npt`, `fix nve_sphere`, `fix nvt_sphere`, `fix npt_asphere`, `fix_modify`

**Default:** none
fix nve command

fix nve/cuda command

Syntax:

fix ID group-ID nve

- ID, group-ID are documented in fix command
- nve = style name of this fix command

Examples:

fix 1 all nve

Description:

Perform constant NVE integration to update position and velocity for atoms in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix nvt, fix npt

Default: none
**fix nve/asphere command**

**Syntax:**

```
fix ID group-ID nve/asphere
```

- ID, group-ID are documented in fix command
- nve/asphere = style name of this fix command

**Examples:**

```
fix 1 all nve/asphere
```

**Description:**

Perform constant NVE integration to update position, velocity, orientation, and angular velocity for aspherical particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

This fix differs from the fix nve command, which assumes point particles and only updates their position and velocity.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

**Related commands:**

- fix nve, fix nve/sphere

**Default:** none
fix nve/asphere/noforce command

Syntax:

fix ID group-ID nve/asphere/noforce

• ID, group-ID are documented in fix command
• nve/asphere/noforce = style name of this fix command

Examples:

fix 1 all nve/asphere/noforce

Description:

Perform updates of position and orientation, but not velocity or angular momentum for atoms in the group each timestep. In other words, the force and torque on the atoms is ignored and their velocity and angular momentum are not updated. The atom velocities and angular momenta are used to update their positions and orientation.

This is useful as an implicit time integrator for Fast Lubrication Dynamics, since the velocity and angular momentum are updated by the pair_style lubricuteU command.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

Related commands:

fix nve/noforce, fix nve/asphere

Default: none
fix nve/eff command

Syntax:

fix ID group-ID nve/eff

- ID, group-ID are documented in fix command
- nve/eff = style name of this fix command

Examples:

fix 1 all nve/eff

Description:

Perform constant NVE integration to update position and velocity for nuclei and electrons in the group for the electron force field model. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

The operation of this fix is exactly like that described by the fix nve command, except that the radius and radial velocity of electrons are also updated.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix nve, fix nvt/eff, fix npt/eff

Default: none
fix nve/limit command

Syntax:

fix ID group-ID nve/limit xmax

- ID, group-ID are documented in fix command
- nve = style name of this fix command
- xmax = maximum distance an atom can move in one timestep (distance units)

Examples:

fix 1 all nve/limit 0.1

Description:

Perform constant NVE updates of position and velocity for atoms in the group each timestep. A limit is imposed on the maximum distance an atom can move in one timestep. This is useful when starting a simulation with a configuration containing highly overlapped atoms. Normally this would generate huge forces which would blow atoms out of the simulation box, causing LAMMPS to stop with an error.

Using this fix can overcome that problem. Forces on atoms must still be computable (which typically means 2 atoms must have a separation distance > 0.0). But large velocities generated by large forces are reset to a value that corresponds to a displacement of length xmax in a single timestep. Xmax is specified in distance units; see the units command for details. The value of xmax should be consistent with the neighbor skin distance and the frequency of neighbor list re-building, so that pairwise interactions are not missed on successive timesteps as atoms move. See the neighbor and neigh_modify commands for details.

Note that if a velocity reset occurs the integrator will not conserve energy. On steps where no velocity resets occur, this integrator is exactly like the fix nve command. Since forces are unaltered, pressures computed by thermodynamic output will still be very large for overlapped configurations.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the count of how many updates of atom's velocity/position were limited by the maximum distance criterion. This should be roughly the number of atoms so affected, except that updates occur at both the beginning and end of a timestep in a velocity Verlet timestepping algorithm. This is a cumulative quantity for the current run, but is re-initialized to zero each time a run is performed. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:
fix nve, fix nve/noforce, pair_style soft

Default: none
fix nve/line command

Syntax:

fix ID group-ID nve/line

• ID, group-ID are documented in fix command
• nve/line = style name of this fix command

Examples:

fix 1 all nve/line

Description:

Perform constant NVE integration to update position, velocity, orientation, and angular velocity for line segment particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

This fix differs from the fix nve command, which assumes point particles and only updates their position and velocity.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that particles be line segments as defined by the atom_style line command.

Related commands:

fix nve, fix nve/asphere

Default: none
fix nve/noforce command

Syntax:

fix ID group-ID nve

- ID, group-ID are documented in fix command
- nve/noforce = style name of this fix command

Examples:

fix 3 wall nve/noforce

Description:

Perform updates of position, but not velocity for atoms in the group each timestep. In other words, the force on the atoms is ignored and their velocity is not updated. The atom velocities are used to update their positions.

This can be useful for wall atoms, when you set their velocities, and want the wall to move (or stay stationary) in a prescribed fashion.

This can also be accomplished via the fix setforce command, but with fix nve/noforce, the forces on the wall atoms are unchanged, and can thus be printed by the dump command or queried with an equal-style variable that uses the fcm() group function to compute the total force on the group of atoms.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix nve

Default: none
**fix nve/sphere command**

**fix nve/sphere/omp command**

**Syntax:**

```latex
fix ID group-ID nve/sphere
```

- ID, group-ID are documented in fix command
- nve/sphere = style name of this fix command
- zero or more keyword/value pairs may be appended
- keyword = update

```latex
update value = dipole
dipole = update orientation of dipole moment during integration
```

**Examples:**

```bash
fix 1 all nve/sphere
fix 1 all nve/sphere update dipole
```

**Description:**

Perform constant NVE integration to update position, velocity, and angular velocity for extended spherical particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

This fix differs from the fix nve command, which assumes point particles and only updates their position and velocity.

If the `update` keyword is used with the `dipole` value, then the orientation of the dipole moment of each particle is also updated during the time integration. This option should be used for models where a dipole moment is assigned to particles via use of the `atom_style dipole` command.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix command-line switch` when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restart, fix_modify, output, run start/stop, minimize info:**
No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the atom_style sphere command. If the dipole keyword is used, then they must also store a dipole moment as defined by the atom_style dipole command.

All particles in the group must be finite-size spheres. They cannot be point particles.

**Related commands:**

fix nve, fix nve/asphere

**Default:** none
**fix nve/tri command**

**Syntax:**

```
fix ID group-ID nve/tri
```

- ID, group-ID are documented in fix command
- nve/tri = style name of this fix command

**Examples:**

```
fix 1 all nve/tri
```

**Description:**

Perform constant NVE integration to update position, velocity, orientation, and angular momentum for triangular particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

This fix differs from the fix nve command, which assumes point particles and only updates their position and velocity.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that particles be triangles as defined by the atom_style tri command.

**Related commands:**

fix nve, fix nve/asphere

**Default:** none
fix nvt/asphere command

Syntax:

fix ID group-ID nvt/asphere keyword value ...

- ID, group-ID are documented in fix command
- nvt/asphere = style name of this fix command
- additional thermostat related keyword/value pairs from the fix nvt command can be appended

Examples:

fix 1 all nvt/asphere temp 300.0 300.0 100.0
drag 0.2

Description:

Perform constant NVT integration to update position, velocity, orientation, and angular velocity each timestep for aspherical or ellipsoidal particles in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This fix differs from the fix nvt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the aspherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostating takes place; see the description below.

Additional parameters affecting the thermostat are specified by keywords and values documented with the fix nvt command. See, for example, discussion of the \textit{temp} and \textit{drag} keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/asphere", as if this command had been issued:

compute fix-ID_temp group-ID temp/asphere

See the compute temp/asphere command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = \textit{thermo_temp}. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of \textit{thermo_temp} will have no effect on this fix.

Like other fixes that perform thermostating, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute
commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostating is performed on the remaining thermal degrees of freedom, and the bias is added back in.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the state of the Nose/Hoover thermostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The **fix_modify temp** option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used in its thermostating procedure.

The **fix_modify energy** option is supported by this fix to add the energy change induced by Nose/Hoover thermostating to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the **fix nvt** command.

This fix can ramp its target temperature over multiple runs, using the **start** and **stop** keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momentum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

**Related commands:**

fix nvt, fix nve_asphere, fix npt_asphere, fix_modify

**Default:** none
fix nvt/sllod command

Syntax:

fix ID group-ID nvt/sllod keyword value ...

- ID, group-ID are documented in fix command
- nvt/sllod = style name of this fix command
- additional thermostat related keyword/value pairs from the fix nvt command can be appended

Examples:

fix 1 all nvt/sllod temp 300.0 300.0 100.0
fix 1 all nvt/sllod temp 300.0 300.0 100.0 drag 0.2

Description:

Perform constant NVT integration to update positions and velocities each timestep for atoms in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This thermostat is used for a simulation box that is changing size and/or shape, for example in a non-equilibrium MD (NEMD) simulation. The size/shape change is induced by use of the fix deform command, so each point in the simulation box can be thought of as having a "streaming" velocity. This position-dependent streaming velocity is subtracted from each atom's actual velocity to yield a thermal velocity which is used for temperature computation and thermostatting. For example, if the box is being sheared in x, relative to y, then points at the bottom of the box (low y) have a small x velocity, while points at the top of the box (hi y) have a large x velocity. These velocities do not contribute to the thermal "temperature" of the atom.

IMPORTANT NOTE: Fix deform has an option for remapping either atom coordinates or velocities to the changing simulation box. To use fix nvt/sllod, fix deform should NOT remap atom positions, because fix nvt/sllod adjusts the atom positions and velocities to create a velocity profile that matches the changing box size/shape. Fix deform SHOULD remap atom velocities when atoms cross periodic boundaries since that is consistent with maintaining the velocity profile created by fix nvt/sllod. LAMMPS will give an error if this setting is not consistent.

The SLLOD equations of motion coupled to a Nose/Hoover thermostat are discussed in (Tuckerman) (eqs 4 and 5), which is what is implemented in LAMMPS in a velocity Verlet formulation.

Additional parameters affecting the thermostat are specified by keywords and values documented with the fix nvt command. See, for example, discussion of the temp and drag keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/deform", as if this command had been issued:

compute fix-ID_temp group-ID temp/deform

See the compute temp/deform command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.
Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = thermo_temp. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of thermo_temp will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the state of the Nose/Hoover thermostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify temp option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used in its thermostatting procedure.

The fix_modify energy option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nvt command.

This fix can ramp its target temperature over multiple runs, using the start and stop keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

**Restrictions:**

This fix works best without Nose-Hoover chain thermostats, i.e. using tchain = 1. Setting tchain to larger values can result in poor equilibration.

**Related commands:**

fix nve, fix nvt, fix temp/rescale, fix langevin, fix_modify, compute temp/deform

**Default:**

Same as fix nvt, except tchain = 1.

fix nvt/sllod/eff command

Syntax:

fix ID group-ID nvt/sllod/eff keyword value ...

- ID, group-ID are documented in fix command
- nvt/sllod/eff = style name of this fix command
- additional thermostat related keyword/value pairs from the fix nvt/eff command can be appended

Examples:

fix 1 all nvt/sllod/eff temp 300.0 300.0 0.1
fix 1 all nvt/sllod/eff temp 300.0 300.0 0.1 drag 0.2

Description:

Perform constant NVT integration to update positions and velocities each timestep for nuclei and electrons in the group for the electron force field model, using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

The operation of this fix is exactly like that described by the fix nvt/sllod command, except that the radius and radial velocity of electrons are also updated and thermostatted. Likewise the temperature calculated by the fix, using the compute it creates (as discussed in the fix nvt, npt, and nph doc page), is performed with a compute temp/deform/eff command that includes the eFF contribution to the temperature from the electron radial velocity.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify temp option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used in its thermostatting procedure.

The fix_modify energy option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nvt/eff command.

This fix can ramp its target temperature over multiple runs, using the start and stop keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.
This fix works best without Nose-Hoover chain thermostats, i.e. using $t_{\text{chain}} = 1$. Setting $t_{\text{chain}}$ to larger values can result in poor equilibration.

**Related commands:**

- `fix nve/eff`, `fix nvt/eff`, `fix langevin/eff`, `fix nvt/sllod`, `fix_modify`, `compute temp/deform/eff`

**Default:**

Same as `fix nvt/eff`, except $t_{\text{chain}} = 1$.

---

**fix nvt/sphere command**

**Syntax:**

```
fix ID group-ID nvt/sphere keyword value ...
```

- ID, group-ID are documented in fix command
- nvt/sphere = style name of this fix command
- additional thermostat related keyword/value pairs from the fix nvt command can be appended

**Examples:**

```
fix 1 all nvt/sphere temp 300.0 300.0 100.0
fix 1 all nvt/sphere temp 300.0 300.0 100.0 drag 0.2
```

**Description:**

Perform constant NVT integration to update position, velocity, and angular velocity each timestep for extended spherical particles in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This fix differs from the fix nvt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the spherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostating takes place; see the description below.

Additional parameters affecting the thermostat are specified by keywords and values documented with the fix nvt command. See, for example, discussion of the temp and drag keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/sphere", as if this command had been issued:

```
compute fix-ID_temp group-ID temp/sphere
```

See the compute temp/sphere command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = thermo_temp. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of thermo_temp will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute
commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostattion is performed on the remaining thermal degrees of freedom, and the bias is added back in.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the state of the Nose/Hoover thermostat to **binary restart files**. See the `read_restart` command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The **fix_modify temp** option is supported by this fix. You can use it to assign a **compute** you have defined to this fix which will be used in its thermostattion procedure.

The **fix_modify energy** option is supported by this fix to add the energy change induced by Nose/Hoover thermostattion to the system’s potential energy as part of **thermodynamic output**.

This fix computes the same global scalar and global vector of quantities as does the `fix nvt` command.

This fix can ramp its target temperature over multiple runs, using the **start** and **stop** keywords of the `run` command. See the `run` command for details of how to do this.

This fix is not invoked during **energy minimization**.

**Restrictions:**

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the **atom_style sphere** command.

All particles in the group must be finite-size spheres. They cannot be point particles.

**Related commands:**

`fix nvt`, `fix nve_sphere`, `fix nvt_asphere`, `fix npt_sphere`, `fix_modify`

**Default:** none
fix orient/fcc command

fix ID group-ID orient/fcc nstats dir alat dE cutlo cuthi file0 file1

- ID, group-ID are documented in fix command
- nstats = print stats every this many steps, 0 = never
- dir = 0/1 for which crystal is used as reference
- alat = fcc cubic lattice constant (distance units)
- dE = energy added to each atom (energy units)
- cutlo, cuthi = values between 0.0 and 1.0, cutlo < cuthi
- file0, file1 = files that specify orientation of each grain

Examples:

fix gb all orient/fcc 0 1 4.032008 0.001 0.25 0.75 xi.vec chi.vec

Description:

The fix applies an orientation-dependent force to atoms near a planar grain boundary which can be used to induce grain boundary migration (in the direction perpendicular to the grain boundary plane). The motivation and explanation of this force and its application are described in (Janssens). The force is only applied to atoms in the fix group.

The basic idea is that atoms in one grain (on one side of the boundary) have a potential energy dE added to them. Atoms in the other grain have 0.0 potential energy added. Atoms near the boundary (whose neighbor environment is intermediate between the two grain orientations) have an energy between 0.0 and dE added. This creates an effective driving force to reduce the potential energy of atoms near the boundary by pushing them towards one of the grain orientations. For dir = 1 and dE > 0, the boundary will thus move so that the grain described by file0 grows and the grain described by file1 shrinks. Thus this fix is designed for simulations of two-grain systems, either with one grain boundary and free surfaces parallel to the boundary, or a system with periodic boundary conditions and two equal and opposite grain boundaries. In either case, the entire system can displace during the simulation, and such motion should be accounted for in measuring the grain boundary velocity.

The potential energy added to atom I is given by these formulas
The order parameter $\xi_i$ for atom $I$ in equation (1) is a sum over the 12 nearest neighbors of atom $I$. $R_j$ is the vector from atom $I$ to its neighbor $J$, and $R_{IJ}$ is a vector in the reference (perfect) crystal. That is, if $\text{dir} = 0/1$, then $R_{IJ}$ is a vector to an atom coord from file 0/1. Equation (2) gives the expected value of the order parameter $\xi_{IJ}$ in the other grain. Hi and lo cutoffs are defined in equations (3) and (4), using the input parameters $\text{cutlo}$ and $\text{cuthi}$ as thresholds to avoid adding grain boundary energy when the deviation in the order parameter from 0 or 1 is small (e.g. due to thermal fluctuations in a perfect crystal). The added potential energy $U_i$ for atom $I$ is given in equation (6) where it is interpolated between 0 and $dE$ using the two threshold $\xi_i$ values and the $\text{Wi}$ value of equation (5).

\[
\xi_i = \sum_{j=1}^{12} |r_j - r_j^I| \tag{1}
\]

\[
\xi_{IJ} = \sum_{j=1}^{12} |r_j^J - r_j^I| \tag{2}
\]

\[
\xi_{\text{low}} = \text{cutlo} \xi_{IJ} \tag{3}
\]

\[
\xi_{\text{high}} = \text{cuthi} \xi_{IJ} \tag{4}
\]

\[
\omega_i = \frac{\pi}{2} \frac{\xi_i - \xi_{\text{low}}}{\xi_{\text{high}} - \xi_{\text{low}}} \tag{5}
\]

\[
u_i = \begin{cases} 
0 & \text{for } \xi_i < \xi_{\text{low}} \\
\text{dE} \frac{1 - \cos(2\omega_i)}{2} & \text{for } \xi_{\text{low}} < \xi_i < \xi_{\text{high}} \\
\text{dE} & \text{for } \xi_{\text{high}} < \xi_i
\end{cases} \tag{6}
\]

which are fully explained in (Janssens). The order parameter $\xi_i$ for atom $I$ in equation (1) is a sum over the 12 nearest neighbors of atom $I$. $R_j$ is the vector from atom $I$ to its neighbor $J$, and $R_{IJ}$ is a vector in the reference (perfect) crystal. That is, if $\text{dir} = 0/1$, then $R_{IJ}$ is a vector to an atom coord from file 0/1. Equation (2) gives the expected value of the order parameter $\xi_{IJ}$ in the other grain. Hi and lo cutoffs are defined in equations (3) and (4), using the input parameters $\text{cutlo}$ and $\text{cuthi}$ as thresholds to avoid adding grain boundary energy when the deviation in the order parameter from 0 or 1 is small (e.g. due to thermal fluctuations in a perfect crystal). The added potential energy $U_i$ for atom $I$ is given in equation (6) where it is interpolated between 0 and $dE$ using the two threshold $\xi_i$ values and the $\text{Wi}$ value of equation (5).

The derivative of this energy expression gives the force on each atom which thus depends on the orientation of its neighbors relative to the 2 grain orientations. Only atoms near the grain boundary feel a net force which tends to drive them to one of the two grain orientations.

In equation (1), the reference vector used for each neighbor is the reference vector closest to the actual neighbor position. This means it is possible two different neighbors will use the same reference vector. In such cases, the atom in question is far from a perfect orientation and will likely receive the full $dE$ addition, so the effect of duplicate reference vector usage is small.
The *dir* parameter determines which grain wants to grow at the expense of the other. A value of 0 means the first grain will shrink; a value of 1 means it will grow. This assumes that *dE* is positive. The reverse will be true if *dE* is negative.

The *alat* parameter is the cubic lattice constant for the fcc material and is only used to compute a cutoff distance of $1.57 \times \text{alat} / \sqrt{2}$ for finding the 12 nearest neighbors of each atom (which should be valid for an fcc crystal). A longer/shorter cutoff can be imposed by adjusting *alat*. If a particular atom has less than 12 neighbors within the cutoff, the order parameter of equation (1) is effectively multiplied by 12 divided by the actual number of neighbors within the cutoff.

The *dE* parameter is the maximum amount of additional energy added to each atom in the grain which wants to shrink.

The *cutlo* and *cuthi* parameters are used to reduce the force added to bulk atoms in each grain far away from the boundary. An atom in the bulk surrounded by neighbors at the ideal grain orientation would compute an order parameter of 0 or 1 and have no force added. However, thermal vibrations in the solid will cause the order parameters to be greater than 0 or less than 1. The cutoff parameters mask this effect, allowing forces to only be added to atoms with order-parameters between the cutoff values.

*File0* and *file1* are filenames for the two grains which each contain 6 vectors (6 lines with 3 values per line) which specify the grain orientations. Each vector is a displacement from a central atom (0,0,0) to a nearest neighbor atom in an fcc lattice at the proper orientation. The vector lengths should all be identical since an fcc lattice has a coordination number of 12. Only 6 are listed due to symmetry, so the list must include one from each pair of equal-and-opposite neighbors. A pair of orientation files for a Sigma=5 tilt boundary are show below.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files.

The *fix_modify energy* option is supported by this fix to add the potential energy of atom interactions with the grain boundary driving force to the system's potential energy as part of thermodynamic output.

This fix calculates a global scalar which can be accessed by various output commands. The scalar is the potential energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix also calculates a per-atom array which can be accessed by various output commands. The array stores the order parameter $X_i$ and normalized order parameter (0 to 1) for each atom. The per-atom values can be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the *run* command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix should only be used with fcc lattices.

**Related commands:**

*fix_modify*

**Default:** none
For illustration purposes, here are example files that specify a Sigma=5 tilt boundary. This is for a lattice constant of 3.5706 Angs.

file0:

```
0.798410432046075  1.785300000000000  1.596820864092150
-0.798410432046075  1.785300000000000 -1.596820864092150
2.395231296138225   0.000000000000000  0.798410432046075
0.798410432046075   0.000000000000000 -2.395231296138225
1.596820864092150   1.785300000000000 -0.798410432046075
1.596820864092150  -1.785300000000000 -0.798410432046075
```

file1:

```
-0.798410432046075  1.785300000000000  1.596820864092150
0.798410432046075   1.785300000000000 -1.596820864092150
0.798410432046075   0.000000000000000  2.395231296138225
2.395231296138225   0.000000000000000 -0.798410432046075
1.596820864092150   1.785300000000000  0.798410432046075
1.596820864092150  -1.785300000000000  0.798410432046075
```
fix planeforce command

Syntax:

fix ID group-ID planeforce x y z

• ID, group-ID are documented in fix command
• lineforce = style name of this fix command
• x y z = 3-vector that is normal to the plane

Examples:

fix hold boundary planeforce 1.0 0.0 0.0

Description:

Adjust the forces on each atom in the group so that only the components of force in the plane specified by the normal vector \((x,y,z)\) remain. This is done by subtracting out the component of force perpendicular to the plane.

If the initial velocity of the atom is 0.0 (or in the plane), then it should continue to move in the plane thereafter.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

Restrictions: none

Related commands:

fix lineforce

Default: none
fix poems

Syntax:

fix ID group-ID poems keyword values

- ID, group-ID are documented in fix command
- poems = style name of this fix command
- keyword = group or file or molecule

  group values = list of group IDs
  molecule values = none
  file values = filename

Examples:

fix 3 fluid poems group clump1 clump2 clump3
fix 3 fluid poems file cluster.list

Description:

Treats one or more sets of atoms as coupled rigid bodies. This means that each timestep the total force and torque on each rigid body is computed and the coordinates and velocities of the atoms are updated so that the collection of bodies move as a coupled set. This can be useful for treating a large biomolecule as a collection of connected, coarse-grained particles.

The coupling, associated motion constraints, and time integration is performed by the software package Parallelizable Open source Efficient Multibody Software (POEMS) which computes the constrained rigid-body motion of articulated (jointed) multibody systems (Anderson). POEMS was written and is distributed by Prof Kurt Anderson, his graduate student Rudranarayan Mukherjee, and other members of his group at Rensselaer Polytechnic Institute (RPI). Rudranarayan developed the LAMMPS/POEMS interface. For copyright information on POEMS and other details, please refer to the documents in the poems directory distributed with LAMMPS.

This fix updates the positions and velocities of the rigid atoms with a constant-energy time integration, so you should not update the same atoms via other fixes (e.g. nve, nvt, npt, temp/rescale, langevin).

Each body must have a non-degenerate inertia tensor, which means if must contain at least 3 non-collinear atoms. Which atoms are in which bodies can be defined via several options.

For option group, each of the listed groups is treated as a rigid body. Note that only atoms that are also in the fix group are included in each rigid body.

For option molecule, each set of atoms in the group with a different molecule ID is treated as a rigid body.

For option file, sets of atoms are read from the specified file and each set is treated as a rigid body. Each line of the file specifies a rigid body in the following format:

ID type atom1-ID atom2-ID atom3-ID ...

ID as an integer from 1 to M (the number of rigid bodies). Type is any integer; it is not used by the fix poems command. The remaining arguments are IDs of atoms in the rigid body, each typically from 1 to N (the number of
atoms in the system). Only atoms that are also in the fix group are included in each rigid body. Blank lines and lines that begin with '#' are skipped.

A connection between a pair of rigid bodies is inferred if one atom is common to both bodies. The POEMS solver treats that atom as a spherical joint with 3 degrees of freedom. Currently, a collection of bodies can only be connected by joints as a linear chain. The entire collection of rigid bodies can represent one or more chains. Other connection topologies (tree, ring) are not allowed, but will be added later. Note that if no joints exist, it is more efficient to use the fix rigid command to simulate the system.

When the poems fix is defined, it will print out statistics on the total # of clusters, bodies, joints, atoms involved. A cluster in this context means a set of rigid bodies connected by joints.

For computational efficiency, you should turn off pairwise and bond interactions within each rigid body, as they no longer contribute to the motion. The "neigh_modify exclude" and "delete_bonds" commands can be used to do this if each rigid body is a group.

For computational efficiency, you should only define one fix poems which includes all the desired rigid bodies. LAMMPS will allow multiple poems fixes to be defined, but it is more expensive.

The degrees-of-freedom removed by coupled rigid bodies are accounted for in temperature and pressure computations. Similarly, the rigid body contribution to the pressure virial is also accounted for. The latter is only correct if forces within the bodies have been turned off, and there is only a single fix poems defined.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the POEMS package. It is only enabled if LAMMPS was built with that package, which also requires the POEMS library be built and linked with LAMMPS. See the Making LAMMPS section for more info.

**Related commands:**

fix rigid, delete_bonds, neigh_modify exclude

**Default:** none

fix pour command

Syntax:

fix ID group-ID pour N type seed keyword values ...

- ID, group-ID are documented in fix command
- pour = style name of this fix command
- N = # of atoms to insert
- type = atom type to assign to inserted atoms
- seed = random # seed (positive integer)
- one or more keyword/value pairs may be appended to args
- keyword = region or diam or dens or vol or rate or vel

region value = region-ID
  region-ID = ID of region to use as insertion volume
diam values = lo hi
  lo,hi = range of diameters for inserted particles (distance units)
dens values = lo hi
  lo,hi = range of densities for inserted particles
vol values = fraction Nattempt
  fraction = desired volume fraction for filling insertion volume
  Nattempt = max # of insertion attempts per atom
rate value = V
  V = z velocity (3d) or y velocity (2d) at which
  insertion volume moves (velocity units)
vel values (3d) = vxlo vxhi vylo vyhi vz
  vxlo,vxhi = range of x velocities for inserted particles (velocity units)
  vylo,vyhi = range of y velocities for inserted particles (velocity units)
  vz = z velocity (3d) assigned to inserted particles (velocity units)
vel values (2d) = vxlo vxhi vy
  vy = y velocity (2d) assigned to inserted particles (velocity units)

Examples:

fix 3 all pour 1000 2 29494 region myblock
fix 2 all pour 10000 1 19985583 region disk vol 0.33 100 rate 1.0 diam 0.9 1.1

Description:

Insert particles into a granular run every few timesteps within a specified region until N particles have been inserted. This is useful for simulating the pouring of particles into a container under the influence of gravity.

Inserted particles are assigned the specified atom type and are assigned to two groups: the default group "all" and the group specified in the fix pour command (which can also be "all").

This command must use the region keyword to define an insertion volume. The specified region must have been previously defined with a region command. It must be of type block or a z-axis cylinder and must be defined with side = in. The cylinder style of region can only be used with 3d simulations.

Each timestep particles are inserted, they are placed randomly inside the insertion volume so as to mimic a stream of poured particles. The larger the volume, the more particles that can be inserted at any one timestep. Particles are inserted again after enough time has elapsed that the previously inserted particles fall out of the insertion volume under the influence of gravity. Insertions continue every so many timesteps until the desired # of particles
has been inserted.

All other keywords are optional with defaults as shown below. The diam, dens, and vel options enable inserted particles to have a range of diameters or densities or xy velocities. The specific values for a particular inserted particle will be chosen randomly and uniformly between the specified bounds. The vz or vy value for option vel assigns a z-velocity (3d) or y-velocity (2d) to each inserted particle.

The vol option specifies what volume fraction of the insertion volume will be filled with particles. The higher the value, the more particles are inserted each timestep. Since inserted particles cannot overlap, the maximum volume fraction should be no higher than about 0.6. Each timestep particles are inserted, LAMMPS will make up to a total of M tries to insert the new particles without overlaps, where M = # of inserted particles * Nattempt. If LAMMPS is unsuccessful at completing all insertions, it prints a warning.

The rate option moves the insertion volume in the z direction (3d) or y direction (2d). This enables pouring particles from a successively higher height over time.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. This means you must be careful when restarting a pouring simulation, when the restart file was written in the middle of the pouring operation. Specifically, you should use a new fix pour command in the input script for the restarted simulation that continues the operation. You will need to adjust the arguments of the original fix pour command to do this.

Also note that because the state of the random number generator is not saved in restart files, you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior if you adjust the fix pour parameters appropriately.

None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

For 3d simulations, a gravity fix in the -z direction must be defined for use in conjunction with this fix. For 2d simulations, gravity must be defined in the -y direction.

The specified insertion region cannot be a "dynamic" region, as defined by the region command.

**Related commands:**

fix_deposit, fix_gravity, region

**Default:**

The option defaults are diam = 1.0 1.0, dens = 1.0 1.0, vol = 0.25 50, rate = 0.0, vel = 0.0 0.0 0.0 0.0 0.0.
fix press/berendsen command

Syntax:

fix ID group-ID press/berendsen keyword value ...

- ID, group-ID are documented in fix command
- press/berendsen = style name of this fix command

one or more keyword value pairs may be appended

<table>
<thead>
<tr>
<th>Keyword</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>iso</td>
<td>Pstart Pstop Pdamp</td>
</tr>
<tr>
<td>aniso</td>
<td>values = Pstart Pstop Pdamp</td>
</tr>
<tr>
<td>x</td>
<td>or y or z values = Pstart Pstop Pdamp</td>
</tr>
<tr>
<td>couple</td>
<td>= none or xyz or xy or yz or xz</td>
</tr>
<tr>
<td>modulus</td>
<td>value = bulk modulus of system (pressure units)</td>
</tr>
<tr>
<td>dilate</td>
<td>value = all or partial</td>
</tr>
</tbody>
</table>

Examples:

fix 1 all press/berendsen iso 0.0 0.0 1000.0
fix 2 all press/berendsen aniso 0.0 0.0 1000.0 dilate partial

Description:

Reset the pressure of the system by using a Berendsen barostat (Berendsen), which rescales the system volume and (optionally) the atoms coordinates within the simulation box every timestep.

Regardless of what atoms are in the fix group, a global pressure is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword dilate is specified with a value of partial, in which case only the atoms in the fix group are re-scaled. The latter can be useful for leaving the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

IMPORTANT NOTE: Unlike the fix npt or fix nph commands which perform Nose/Hoover barostatting AND time integration, this fix does NOT perform time integration. It only modifies the box size and atom coordinates to effect barostatting. Thus you must use a separate time integration fix, like fix nve or fix nvt to actually update the positions and velocities of atoms. This fix can be used in conjunction with thermostatting fixes to control the temperature, such as fix nvt or fix langevin or fix temp/berendsen.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting and barostatting.

The barostat is specified using one or more of the iso, aniso, x, y, z, and couple keywords. These keywords give you the ability to specify the 3 diagonal components of an external stress tensor, and to couple various of these components together so that the dimensions they represent are varied together during a constant-pressure simulation. Unlike the fix npt and fix nph commands, this fix cannot be used with triclinic (non-orthogonal) simulation boxes to control all 6 components of the general pressure tensor.
The target pressures for each of the 3 diagonal components of the stress tensor can be specified independently via the $x$, $y$, $z$, keywords, which correspond to the 3 simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a ramped value during the run from $P_{start}$ to $P_{stop}$. If a target pressure is specified for a component, then the corresponding box dimension will change during a simulation. For example, if the $y$ keyword is used, the $y$-box length will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the `fix deform` command.

For all barostat keywords, the $P_{damp}$ parameter determines the time scale on which pressure is relaxed. For example, a value of 1000.0 means to relax the pressure in a timespan of (roughly) 1000 time units (tau or fmsec or psec - see the `units` command).

IMPORTANT NOTE: The relaxation time is actually also a function of the bulk modulus of the system (inverse of isothermal compressibility). The bulk modulus has units of pressure and is the amount of pressure that would need to be applied (isotropically) to reduce the volume of the system by a factor of 2 (assuming the bulk modulus was a constant, independent of density, which it's not). The bulk modulus can be set via the keyword `modulus`. The $P_{damp}$ parameter is effectively multiplied by the bulk modulus, so if the pressure is relaxing faster than expected or desired, increasing the bulk modulus has the same effect as increasing $P_{damp}$. The converse is also true. LAMMPS does not attempt to guess a correct value of the bulk modulus; it just uses 10.0 as a default value which gives reasonable relaxation for a Lennard-Jones liquid, but will be way off for other materials and way too small for solids. Thus you should experiment to find appropriate values of $P_{damp}$ and/or the `modulus` when using this fix.

The `couple` keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, $xz$ means the $P_{xx}$ and $P_{zz}$ components of the stress tensor are coupled. $XYZ$ means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The $P_{start}$, $P_{stop}$, $P_{damp}$ parameters for any coupled dimensions must be identical. `Couple xyz` can be used for a 2d simulation; the $z$ dimension is simply ignored.

The `iso` and `aniso` keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword `iso` means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso $P_{start}$ $P_{stop}$ $P_{damp}$" is the same as specifying these 4 keywords:

```plaintext
x $P_{start}$ $P_{stop}$ $P_{damp}$
y $P_{start}$ $P_{stop}$ $P_{damp}$
z $P_{start}$ $P_{stop}$ $P_{damp}$
couple $xyz$
```

The keyword `aniso` means $x$, $y$, and $z$ dimensions are controlled independently using the $P_{xx}$, $P_{yy}$, and $P_{zz}$ components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso $P_{start}$ $P_{stop}$ $P_{damp}$" is the same as specifying these 4 keywords:

```plaintext
x $P_{start}$ $P_{stop}$ $P_{damp}$
y $P_{start}$ $P_{stop}$ $P_{damp}$
z $P_{start}$ $P_{stop}$ $P_{damp}$
couple $none$
```

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style
"temp" and "pressure", as if these commands had been issued:

```plaintext
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp
```

See the `compute temp` and `compute pressure` commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is the same as the fix group.

Note that these are NOT the computes used by thermodynamic output (see the `thermo_style` command) with ID = 
`thermo_temp` and `thermo_press`. This means you can change the attributes of this fix's temperature or pressure via 
the `compute_modify` command or print this temperature or pressure during thermodynamic output via the 
`thermo_style custom` command using the appropriate compute-ID. It also means that changing attributes of 
`thermo_temp` or `thermo_press` will have no effect on this fix.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files.

The `fix_modify temp` and `press` options are supported by this fix. You can use them to assign a compute you have 
defined to this fix which will be used in its temperature and pressure calculations. If you do this, note that the 
kinetic energy derived from the compute temperature should be consistent with the virial term computed using all 
atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

No global or per-atom quantities are stored by this fix for access by various `output commands`.

This fix can ramp its target pressure over multiple runs, using the `start` and `stop` keywords of the `run` command. 
See the `run` command for details of how to do this.

This fix is not invoked during energy minimization.

**Restrictions:**

Any dimension being adjusted by this fix must be periodic.

**Related commands:**

`fix nve`, `fix nph`, `fix npt`, `fix temp/berendsen`, `fix_modify`

**Default:**

The keyword defaults are dilate = all, modulus = 10.0 in units of pressure for whatever units are defined.

fix print command

Syntax:

fix ID group-ID print N string keyword value ... 

- ID, group-ID are documented in fix command 
- print = style name of this fix command 
- N = print every N steps 
- string = text string to print with optional variable names 
- zero or more keyword/value pairs may be appended 
- keyword = file or append or screen or title 

  file value = filename 
  append value = filename 
  screen value = yes or no 
  title value = string 
    string = text to print as 1st line of output file 

Examples:

fix extra all print 100 "Coords of marker atom = $x $y $z"
fix extra all print 100 "Coords of marker atom = $x $y $z" file coord.txt 

Description:

Print a text string every N steps during a simulation run. This can be used for diagnostic purposes or as a 
debugging tool to monitor some quantity during a run. The text string must be a single argument, so it should be 
enclosed in double quotes if it is more than one word. If it contains variables it must be enclosed in double quotes 
to insure they are not evaluated when the input script line is read, but will instead be evaluated each time the 
string is printed.

See the variable command for a description of equal style variables which are the most useful ones to use with the 
fix print command, since they are evaluated afresh each timestep that the fix print line is output. Equal-style 
variables calculate formulas involving mathematical operations, atom properties, group properties, 
thermodynamic properties, global values calculated by a compute or fix, or references to other variables.

If the file or append keyword is used, a filename is specified to which the output generated by this fix will be 
written. If file is used, then the filename is overwritten if it already exists. If append is used, then the filename is 
appended to if it already exists, or created if it does not exist.

If the screen keyword is used, output by this fix to the screen and logfile can be turned on or off as desired.

The title keyword allow specification of the string that will be printed as the first line of the output file, assuming 
the file keyword was used. By default, the title line is as follows:

# Fix print output for fix ID 

where ID is replaced with the fix-ID.

Restart, fix_modify, output, run start/stop, minimize info:
No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

variable, print

**Default:**

The option defaults are no file output, screen = yes, and title string as described above.
fix qeq/comb command

fix qeq/comb/omp command

Syntax:

```
fix ID group-ID qeq/comb Nevery precision keyword value ...
```

- ID, group-ID are documented in fix command
- qeq/comb = style name of this fix command
- Nevery = perform charge equilibration every this many steps
- precision = convergence criterion for charge equilibration
- zero or more keyword/value pairs may be appended
- keyword = file
  
  ```
  file value = filename
  filename = name of file to write QEQ equilibration info to
  ```

Examples:

```
fix 1 surface qeq/comb 10 0.0001
```

Description:

Perform charge equilibration (QeQ) in conjunction with the COMB (Charge-Optimized Many-Body) potential as described in (COMB_1) and (COMB_2). It performs the charge equilibration portion of the calculation using the so-called QEq method, whereby the charge on each atom is adjusted to minimize the energy of the system. This fix can only be used with the COMB potential; see the fix qeq/reax command for a QeQ calculation that can be used with any potential.

Only charges on the atoms in the specified group are equilibrated. The fix relies on the pair style (COMB in this case) to calculate the per-atom electronegativity (effective force on the charges). An electronegativity equalization calculation (or QEq) is performed in an interactive fashion, which in parallel requires communication at each iteration for processors to exchange charge information about nearby atoms with each other. See Rappe_and_Goddard and Rick_and_Stuart for details.

During a run, charge equilibration is performed every Nevery time steps. Charge equilibration is also always enforced on the first step of each run. The precision argument controls the tolerance for the difference in electronegativity for all atoms during charge equilibration. Precision is a trade-off between the cost of performing charge equilibration (more iterations) and accuracy.

If the file keyword is used, then information about each equilibration calculation is written to the specified file.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.
You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix produces a per-atom vector which can be accessed by various output commands. The vector stores the gradient of the charge on each atom. The per-atom values be accessed on any timestep.

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix command currently only supports pair style comb.

**Related commands:**

pair_style comb

**Default:**

No file output is performed.

---


fix qeq/reax command

Syntax:

```plaintext
fix ID group-ID qeq/reax Nevery cutlo cuthi tolerance params
```

- `ID, group-ID` are documented in fix command
- `qeq/reax` = style name of this fix command
- `Nevery` = perform QEq every this many steps
- `cutlo, cuthi` = lo and hi cutoff for Taper radius
- `tolerance` = precision to which charges will be equilibrated
- `params` = reax/c or a filename

Examples:

```plaintext
fix 1 all qeq/reax 1 0.0 10.0 1.0e-6 reax/c
fix 1 all qeq/reax 1 0.0 10.0 1.0e-6 param.qeq
```

Description:

Perform the charge equilibration (QEq) method as described in (Rappe and Goddard) and formulated in (Nakano). It is typically used in conjunction with the ReaxFF force field model as implemented in the `pair_style reax/c` command, but it can be used with any potential in LAMMPS, so long as it defines and uses charges on each atom. The `fix qeq/comb` command should be used to perform charge equilibration with the COMB potential. For more technical details about the charge equilibration performed by fix qeq/reax, see the (Aktulga) paper.

The QEq method minimizes the electrostatic energy of the system by adjusting the partial charge on individual atoms based on interactions with their neighbors. It requires some parameters for each atom type. If the `params` setting above is the word "reax/c", then these are extracted from the `pair_style reax/c` command and the ReaxFF force field file it reads in. If a file name is specified for `params`, then the parameters are taken from the specified file and the file must contain one line for each atom type. The latter form must be used when performing QeQ with a non-ReaxFF potential. Each line should be formatted as follows:

```plaintext
itype chi eta gamma
```

where `itype` is the atom type from 1 to Ntypes, `chi` denotes the electronegativity in eV, `eta` denotes the self-Coulomb potential in eV, and `gamma` denotes the valence orbital exponent. Note that these 3 quantities are also in the ReaxFF potential file, except that `eta` is defined here as twice the `eta` value in the ReaxFF file. Note that unlike the rest of LAMMPS, the units of this fix are hard-coded to be A, eV, and electronic charge.

Restrictions:
This fix is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix does not correctly handle interactions involving multiple periodic images of the same atom. Hence, it should not be used for periodic cell dimensions less than 10 angstroms.

**Related commands:**

pair_style reax/c

**Default:** none


**fix reax/bonds command**

**Syntax:**

```plaintext
fix ID group-ID reax/bonds Nevery filename
```

- ID, group-ID are documented in `fix` command
- `reax/bonds` = style name of this fix command
- `Neveny` = output interval in timesteps
- `filename` = name of output file

**Examples:**

```plaintext
fix 1 all reax/bonds 100 bonds.tatb
```

**Description:**

Write out the bond information computed by the ReaxFF potential specified by `pair_style reax`. The bond information is written to `filename` on timesteps that are multiples of `Neveny`, including timestep 0.

The format of the output file should be self-explanatory.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the `start/stop` keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

The fix reax/bonds command requires that the `pair_style reax` be invoked. This fix is part of the REAX package. It is only enabled if LAMMPS was built with that package, which also requires the REAX library be built and linked with LAMMPS. See the Making LAMMPS section for more info.

**Related commands:**

- `pair_style reax`, `pair_style reax/c/bonds`

**Default:** none
fix reax/c/bonds command

Syntax:

fix ID group-ID reax/c/bonds Nevery Nrepeat Nfreq filename

- ID, group-ID are documented in fix command
- reax/c/bonds = style name of this command
- Nevery = output interval in timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps
- filename = name of output file

Examples:

fix 1 all reax/c/bonds 10 10 100 bonds.reaxc

Description:

Write out the bond information computed by the ReaxFF potential specified by pair_style reax/c. Bond order values are averaged and the bond information is written to filename on timesteps that are multiples of Nfreq, including timestep 0.

The Nevery, Nrepeat, and Nfreq arguments specify on what timesteps the input values will be used in order to contribute to the average. The final averaged quantities are generated on timesteps that are a multiple of Nfreq. The average is over Nrepeat quantities, computed in the preceding portion of the simulation every Nevery timesteps. Nfreq must be a multiple of Nevery and Nevery must be non-zero even if Nrepeat is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nfreq > (Nrepeat-1)*Nevery is required.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc.

The format of the output file should be self-explanatory. When using the same force field file with pair_style reax and pair_style reax/c, the following commands generate the same bond information:

fix 1 all reax/bonds N bonds.reax
fix 1 all reax/c/bonds 1 1 N bonds.reaxc

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

The fix reax/c/bonds requires that the pair_style reax/c be invoked. This fix is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.
Related commands:

pair_style reax/c, fix reax/bonds

Default: none
fix recenter command

Syntax:

fix ID group-ID recenter x y z keyword value ...

- ID, group-ID are documented in fix command
- recenter = style name of this fix command
- x,y,z = constrain center-of-mass to these coords (distance units), any coord can also be NULL or INIT (see below)
- zero or more keyword/value pairs may be appended
- keyword = shift or units

    shift value = group-ID
    group-ID = group of atoms whose coords are shifted
    units value = box or lattice or fraction

Examples:

fix 1 all recenter 0.0 0.5 0.0
fix 1 all recenter INIT INIT NULL
fix 1 all recenter INIT 0.0 0.0 units box

Description:

Constrain the center-of-mass position of a group of atoms by adjusting the coordinates of the atoms every timestep. This is simply a small shift that does not alter the dynamics of the system or change the relative coordinates of any pair of atoms in the group. This can be used to insure the entire collection of atoms (or a portion of them) do not drift during the simulation due to random perturbations (e.g. fix langevin thermostatting).

Distance units for the x,y,z values are determined by the setting of the units keyword, as discussed below. One or more x,y,z values can also be specified as NULL, which means exclude that dimension from this operation. Or it can be specified as INIT which means to constrain the center-of-mass to its initial value at the beginning of the run.

The center-of-mass (COM) is computed for the group specified by the fix. If the current COM is different than the specified x,y,z, then a group of atoms has their coordinates shifted by the difference. By default the shifted group is also the group specified by the fix. A different group can be shifted by using the shift keyword. For example, the COM could be computed on a protein to keep it in the center of the simulation box. But the entire system (protein + water) could be shifted.

If the units keyword is set to box, then the distance units of x,y,z are defined by the units command - e.g. Angstroms for real units. A lattice value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. A fraction value means a fractional distance between the lo/hi box boundaries, e.g. 0.5 = middle of the box. The default is to use lattice units.

Note that the velocity command can be used to create velocities with zero aggregate linear and/or angular momentum.

IMPORTANT NOTE: This fix performs its operations at the same point in the timestep as other time integration fixes, such as fix nve, fix nvt, or fix npt. Thus fix recenter should normally be the last such fix specified in the
input script, since the adjustments it makes to atom coordinates should come after the changes made by time integration. LAMMPS will warn you if your fixes are not ordered this way.

IMPORTANT NOTE: If you use this fix on a small group of atoms (e.g. a molecule in solvent) without using the shift keyword to adjust the positions of all atoms in the system, then the results can be unpredictable. For example, if the molecule is pushed in one direction by the solvent, its velocity will increase. But its coordinates will be recentered, meaning it is pushed back towards the force. Thus over time, the velocity and temperature of the molecule could become very large (though it won't appear to be moving due to the recentering). If you are thermostating the entire system, then the solvent would be cooled to compensate. A better solution for this simulation scenario is to use the fix spring command to tether the molecule in place.

**Restart, fix modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix should not be used with an x,y,z setting that causes a large shift in the system on the 1st timestep, due to the requested COM being very different from the initial COM. This could cause atoms to be lost, especially in parallel. Instead, use the displace_atoms command, which can be used to move atoms a large distance.

**Related commands:**

fix momentum, velocity

**Default:**

The option defaults are shift = fix group-ID, and units = lattice.
fix restrain command

Syntax:

fix ID group-ID restrain keyword args ...

- ID, group-ID are documented in fix command
- restrain = style name of this fix command
- one or more keyword/arg pairs may be appended
- keyword = bond or angle or dihedral

bond args = atom1 atom2 Kstart Kstop r0
  atom1,atom2 = IDs of 2 atoms in bond
  Kstart,Kstop = restraint coefficients at start/end of run (energy units)
  r0 = equilibrium bond distance (distance units)

angle args = atom1 atom2 atom3 Kstart Kstop theta0
  atom1,atom2,atom3 = IDs of 3 atoms in angle, atom2 = middle atom
  Kstart,Kstop = restraint coefficients at start/end of run (energy units)
  theta0 = equilibrium angle theta (degrees)

Examples:

fix holdem all restrain bond 45 48 2000.0 2000.0 2.75
fix holdem all restrain dihedral 1 2 3 4 2000.0 2000.0 120.0
fix holdem all restrain bond 45 48 2000.0 2000.0 2.75 dihedral 1 2 3 4 2000.0 2000.0 120.0
dihedral 1 2 3 5 0.0 2000.0 -120.0 dihedral 1 2 3 6 0.0 2000.0 0.0

Description:

Restrain the motion of the specified sets of atoms by making them part of a bond or angle or dihedral interaction whose strength can vary over time during a simulation. This is functionally equivalent to creating a bond or angle or dihedral for the same atoms in a data file, as specified by the read_data command, albeit with a time-varying pre-factor coefficient. For the purpose of forcefield parameter-fitting or mapping a molecular potential energy surface, this fix reduces the hassle and risk associated with modifying data files. In other words, use this fix to temporarily force a molecule to adopt a particular conformation. To create a permanent bond or angle or dihedral, you should modify the data file.

The group-ID specified by this fix is ignored.

The second example above applies a restraint to hold the dihedral angle formed by atoms 1, 2, 3, and 4 near 120 degrees using a constant restraint coefficient. The fourth example applies similar restraints to multiple dihedral angles using a restraint coefficient that increases from 0.0 to 2000.0 over the course of the run.

IMPORTANT NOTE: Adding a force to atoms implies a change in their potential energy as they move due to the applied force field. For dynamics via the run command, this energy can be added to the system's potential energy for thermodynamic output (see below). For energy minimization via the minimize command, this energy must be added to the system's potential energy to formulate a self-consistent minimization problem (see below).
In order for a restraint to be effective, the restraint force must typically be significantly larger than the forces associated with conventional forcefield terms. If the restraint is applied during a dynamics run (as opposed to during an energy minimization), a large restraint coefficient can significantly reduce the stable timestep size, especially if the atoms are initially far from the preferred conformation. You may need to experiment to determine what value of K works best for a given application.

For the case of finding a minimum energy structure for a single molecule with particular restratins (e.g. for fitting forcefield parameters or constructing a potential energy surface), commands such as the following may be useful:

```bash
# minimize molecule energy with restraints
velocity all create 600.0 8675309 mom yes rot yes dist gaussian
fix NVE all nve
fix TFIX all langevin 600.0 0.0 100 24601
fix REST all restrain dihedral 2 1 3 8 0.0 5000.0 $angle1 dihedral 3 1 2 9 0.0 5000.0 $angle2
fix_modify REST energy yes
run 10000
fix TFIX all langevin 0.0 0.0 100 24601
fix REST all restrain dihedral 2 1 3 8 5000.0 5000.0 $angle1 dihedral 3 1 2 9 5000.0 5000.0 $angle2
fix_modify REST energy yes
run 10000
# sanity check for convergence
minimize 1e-6 1e-9 100 100000
# report unrestrained energies
unfix REST
run 0
```

The bond keyword applies a bond restraint to the specified atoms using the same functional form used by the bond_style harmonic command. The potential associated with the restraint is

$$E = K(r - r_0)^2$$

with the following coefficients:

- K (energy/distance^2)
- r0 (distance)

K and r0 are specified with the fix. Note that the usual 1/2 factor is included in K.

The angle keyword applies an angle restraint to the specified atoms using the same functional form used by the angle_style harmonic command. The potential associated with the restraint is

$$E = K(\theta - \theta_0)^2$$

with the following coefficients:

- K (energy/radian^2)
- theta0 (degrees)

K and theta0 are specified with the fix. Note that the usual 1/2 factor is included in K.
The *dihedral* keyword applies a dihedral restraint to the specified atoms using a simplified form of the function used by the *dihedral_style charmmp* command. The potential associated with the restraint is

\[ E = K [1 + \cos(n\phi - d)] \]

with the following coefficients:

- K (energy)
- n = 1
- d (degrees) = phi0 + 180

K and phi0 are specified with the fix. Note that the value of n is hard-wired to 1. Also note that the energy will be a minimum when the current dihedral angle phi is equal to phi0.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files.

The *fix_modify energy* option is supported by this fix to add the potential energy associated with this fix to the system's potential energy as part of thermodynamic output.

IMPORTANT NOTE: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the *fix_modify energy* option for this fix.

This fix computes a global scalar, which can be accessed by various output commands. The scalar is the potential energy for all the restraints as discussed above. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the *run* command.

**Restrictions:** none

**Related commands:** none

**Default:** none
fix rigid command

fix rigid/nve command

fix rigid/nvt command

fix rigid/npt command

fix rigid/nph command

Syntax:

fix ID group-ID style bodystyle args keyword values ...

- ID, group-ID are documented in fix command
- style = rigid or rigid/nve or rigid/nvt or rigid/npt or rigid/nph
- bodystyle = single or molecule or group

**single** args = none

**molecule** args = none

**group** args = N groupID1 groupID2 ...

N = # of groups

groupID1, groupID2, ... = list of N group IDs

- zero or more keyword/value pairs may be appended
- keyword = langevin or temp or iso or aniso or x or y or z or couple or tparam or pchain or dilate or force or torque or infile

**langevin** values = Tstart Tstop Tperiod seed

Tstart, Tstop = desired temperature at start/stop of run (temperature units)

Tdamp = temperature damping parameter (time units)

seed = random number seed to use for white noise (positive integer)

**temp** values = Tstart Tstop Tdamp

Tstart, Tstop = desired temperature at start/stop of run (temperature units)

Tdamp = temperature damping parameter (time units)

**iso** or **aniso** values = Pstart Pstop Pdamp

Pstart, Pstop = scalar external pressure at start/end of run (pressure units)

Pdamp = pressure damping parameter (time units)

**x** or **y** or **z** values = Pstart Pstop Pdamp

Pstart, Pstop = external stress tensor component at start/end of run (pressure units)

Pdamp = stress damping parameter (time units)

**couple** = none or xyz or xy or yz or zx

**tparam** values = Tchain Titer Torder

Tchain = length of Nose/Hoover thermostat chain

Titer = number of thermostat iterations performed

Torder = 3 or 5 = Yoshida-Suzuki integration parameters

**pchain** values = Pchain

Pchain = length of the Nose/Hoover thermostat chain coupled with the barostat

**dilate** value = dilate-group-ID

dilate-group-ID = only dilate atoms in this group due to barostat volume changes

**force** values = M xflag yflag zflag

M = which rigid body from 1-Nbody (see asterisk form below)

xflag, yflag, zflag = off/on if component of center-of-mass force is active

**torque** values = M xflag yflag zflag

M = which rigid body from 1-Nbody (see asterisk form below)

xflag, yflag, zflag = off/on if component of center-of-mass torque is active
infile filename
filename = file with per-body values of mass, center-of-mass, moments of inertia

Examples:

fix 1 clump rigid single
fix 1 clump rigid single force 1 off off on langevin 1.0 1.0 1.0 428984
fix 1 polychains rigid/nvt molecule temp 1.0 1.0 5.0
fix 1 polychains rigid molecule force 1*5 off off off force 6*10 off off on
fix 1 fluid rigid group 3 clump1 clump2 clump3 torque * off off off
fix 1 rods rigid/npt molecule temp 300.0 300.0 100.0 iso 0.5 0.5 10.0
fix 1 particles rigid/npt molecule temp 1.0 1.0 5.0 x 0.5 0.5 1.0 z 0.5 0.5 1.0 couple xz
fix 1 water rigid/nph molecule iso 0.5 0.5 1.0

Description:

Treat one or more sets of atoms as independent rigid bodies. This means that each timestep the total force and torque on each rigid body is computed as the sum of the forces and torques on its constituent particles and the coordinates, velocities, and orientations of the atoms in each body are updated so that the body moves and rotates as a single entity.

Examples of large rigid bodies are a large colloidal particle, or portions of a large biomolecule such as a protein.

Example of small rigid bodies are patchy nanoparticles, such as those modeled in this paper by Sharon Glotzer's group, clumps of granular particles, lipid molecules consisting of one or more point dipoles connected to other spheroids or ellipsoids, irregular particles built from line segments (2d) or triangles (3d), and coarse-grain models of nano or colloidal particles consisting of a small number of constituent particles. Note that the fix shake command can also be used to rigidify small molecules of 2, 3, or 4 atoms, e.g. water molecules. That fix treats the constituent atoms as point masses.

These fixes also update the positions and velocities of the atoms in each rigid body via time integration, in the NVE, NVT, NPT, or NPH ensemble, as described below.

IMPORTANT NOTE: You should not update the atoms in rigid bodies via other time-integration fixes (e.g. fix nve, fix nvt, fix npt), or you will be integrating their motion more than once each timestep. When performing a hybrid simulation with some atoms in rigid bodies, and some not, a separate time integration fix like fix nve or fix nvt should be used for the non-rigid particles.

IMPORTANT NOTE: These fixes are overkill if you simply want to hold a collection of atoms stationary or have them move with a constant velocity. A simpler way to hold atoms stationary is to not include those atoms in your time integration fix. E.g. use "fix 1 mobile nve" instead of "fix 1 all nve", where "mobile" is the group of atoms that you want to move. You can move atoms with a constant velocity by assigning them an initial velocity (via the velocity command), setting the force on them to 0.0 (via the fix setforce command), and integrating them as usual (e.g. via the fix nve command).

Each rigid body must have two or more atoms. An atom can belong to at most one rigid body. Which atoms are in which bodies can be defined via several options.

For bodystyle single the entire fix group of atoms is treated as one rigid body.

For bodystyle molecule, each set of atoms in the fix group with a different molecule ID is treated as a rigid body.

For bodystyle group, each of the listed groups is treated as a separate rigid body. Only atoms that are also in the fix group are included in each rigid body.
IMPORTANT NOTE: To compute the initial center-of-mass position and other properties of each rigid body, the image flags for each atom in the body are used to "unwrap" the atom coordinates. Thus you must insure that these image flags are consistent so that the unwrapping creates a valid rigid body (one where the atoms are close together), particularly if the atoms in a single rigid body straddle a periodic boundary. This means the input data file or restart file must define the image flags for each atom consistently or that you have used the set command to specify them correctly. If a dimension is non-periodic then the image flag of each atom must be 0 in that dimension, else an error is generated.

By default, each rigid body is acted on by other atoms which induce an external force and torque on its center of mass, causing it to translate and rotate. Components of the external center-of-mass force and torque can be turned off by the force and torque keywords. This may be useful if you wish a body to rotate but not translate, or vice versa, or if you wish it to rotate or translate continuously unaffected by interactions with other particles. Note that if you expect a rigid body not to move or rotate by using these keywords, you must insure its initial center-of-mass translational or angular velocity is 0.0. Otherwise the initial translational or angular momentum the body has will persist.

An xflag, yflag, or zflag set to off means turn off the component of force or torque in that dimension. A setting of on means turn on the component, which is the default. Which rigid body(s) the settings apply to is determined by the first argument of the force and torque keywords. It can be an integer M from 1 to Nbody, where Nbody is the number of rigid bodies defined. A wild-card asterisk can be used in place of, or in conjunction with, the M argument to set the flags for multiple rigid bodies. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of rigid bodies, then an asterisk with no numeric values means all bodies from 1 to N. A leading asterisk means all bodies from 1 to n (inclusive). A trailing asterisk means all bodies from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that you can use the force or torque keywords as many times as you like. If a particular rigid body has its component flags set multiple times, the settings from the final keyword are used.

For computational efficiency, you may wish to turn off pairwise and bond interactions within each rigid body, as they no longer contribute to the motion. The neigh_modify exclude and delete_bonds commands are used to do this.

For computational efficiency, you should typically define one fix rigid which includes all the desired rigid bodies. LAMMPS will allow multiple rigid fixes to be defined, but it is more expensive.

The constituent particles within a rigid body can be point particles (the default in LAMMPS) or finite-size particles, such as spheres or ellipsoids or line segments or triangles. See the atom_style sphere and ellipsoid and line and tri commands for more details on these kinds of particles. Finite-size particles contribute differently to the moment of inertia of a rigid body than do point particles. Finite-size particles can also experience torque (e.g. due to frictional granular interactions) and have an orientation. These contributions are accounted for by these fixes.

Forces between particles within a body do not contribute to the external force or torque on the body. Thus for computational efficiency, you may wish to turn off pairwise and bond interactions between particles within each rigid body. The neigh_modify exclude and delete_bonds commands are used to do this. For finite-size particles this also means the particles can be highly overlapped when creating the rigid body.

The rigid and rigid/nve styles perform constant NVE time integration. The only difference is that the rigid style uses an integration technique based on Richardson iterations. The rigid/nve style uses the methods described in the paper by Miller, which are thought to provide better energy conservation than an iterative approach.

The rigid/nvt style performs constant NVT integration using a Nose/Hoover thermostat with chains as described originally in (Hoover) and (Martyna), which thermostats both the translational and rotational degrees of freedom.
of the rigid bodies. The rigid-body algorithm used by rigid/nvt is described in the paper by Kamberaj.

The rigid/npt and rigid/nph styles performs constant NPT or NPH integration using a Nose/Hoover barostat with chains. For the NPT case, the same Nose/Hoover thermostat is also used as with rigid/nvt.

The barostat parameters are specified using one or more of the iso, aniso, x, y, z and couple keywords. These keywords give you the ability to specify 3 diagonal components of the external stress tensor, and to couple these components together so that the dimensions they represent are varied together during a constant-pressure simulation. The effects of these keywords are similar to those defined in fix npt/nph

NOTE: Currently the rigid/npt and rigid/nph styles do not support triclinic (non-orthogonal) boxes.

The target pressures for each of the 6 components of the stress tensor can be specified independently via the x, y, z keywords, which correspond to the 3 simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a ramped value during the run from Pstart to Pstop. If a target pressure is specified for a component, then the corresponding box dimension will change during a simulation. For example, if the y keyword is used, the y-box length will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the fix deform command.

For all barostat keywords, the Pdamp parameter operates like the Tdamp parameter, determining the time scale on which pressure is relaxed. For example, a value of 10.0 means to relax the pressure in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the units command).

Regardless of what atoms are in the fix group (the only atoms which are time integrated), a global pressure or stress tensor is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword dilate is specified with a dilate-group-ID for a group that represents a subset of the atoms. This can be useful, for example, to leave the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid. Another example is a system consisting of rigid bodies and point particles where the barostat is only coupled with the rigid bodies. This option should be used with care, since it can be unphysical to dilate some atoms and not others, because it can introduce large, instantaneous displacements between a pair of atoms (one dilated, one not) that are far from the dilation origin.

The couple keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, xz means the Pxx and Pzz components of the stress tensor are coupled. Xyz means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The Pstart, Pstop, Pdamp parameters for any coupled dimensions must be identical. Couple xyz can be used for a 2d simulation; the z dimension is simply ignored.

The iso and aniso keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword iso means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple xyz
The keyword *aniso* means x, y, and z dimensions are controlled independently using the $P_{xx}$, $P_{yy}$, and $P_{zz}$ components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple none
```

The keyword/value option pairs are used in the following ways.

The *langevin* and *temp* and *tparam* keywords perform thermostatting of the rigid bodies, altering both their translational and rotational degrees of freedom. What is meant by "temperature" of a collection of rigid bodies and how it can be monitored via the fix output is discussed below.

The *langevin* keyword applies a Langevin thermostat to the constant NVE time integration performed by either the *rigid* or *rigid/nve* styles. It cannot be used with the *rigid/nvt* style. The desired temperature at each timestep is a ramped value during the run from $T_{start}$ to $T_{stop}$. The $Tdamp$ parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the units command). The random # seed must be a positive integer. The way the Langevin thermostatting operates is explained on the fix langevin doc page.

The *temp* and *tparam* keywords apply a Nose/Hoover thermostat to the NVT time integration performed by the *rigid/nvt* style. They cannot be used with the *rigid* or *rigid/nve* styles. The desired temperature at each timestep is a ramped value during the run from $T_{start}$ to $T_{stop}$. The $Tdamp$ parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the units command).

Nose/Hoover chains are used in conjunction with this thermostat. The *tparam* keyword can optionally be used to change the chain settings used. $T_{chain}$ is the number of thermostats in the Nose Hoover chain. This value, along with $Tdamp$ can be varied to dampen undesirable oscillations in temperature that can occur in a simulation. As a rule of thumb, increasing the chain length should lead to smaller oscillations. The keyword $pchain$ specifies the number of thermostats in the chain thermostatting the barostat degrees of freedom.

IMPORTANT NOTE: There are alternate ways to thermostat a system of rigid bodies. You can use fix langevin to treat the individual particles in the rigid bodies as effectively immersed in an implicit solvent, e.g. a Brownian dynamics model. For hybrid systems with both rigid bodies and solvent particles, you can thermostat only the solvent particles that surround one or more rigid bodies by appropriate choice of groups in the compute and fix commands for temperature and thermostatting. The solvent interactions with the rigid bodies should then effectively thermostat the rigid body temperature as well without use of the Langevin or Nose/Hoover options associated with the fix rigid commands.

The *infile* keyword allows a file of rigid body attributes to be read in from a file, rather then letting LAMMPS compute them. There are 3 such attributes: the total mass of the rigid body, its center-of-mass position, and its 6 moments of inertia. For rigid bodies consisting of point particles or non-overlapping finite-size particles, LAMMPS can compute these values accurately. However, for rigid bodies consisting of finite-size particles which overlap each other, LAMMPS will ignore the overlaps when computing these 3 attributes. The amount of error this induces depends on the amount of overlap. To avoid this issue, the values can be pre-computed (e.g. using Monte Carlo integration).

The format of the file is as follows. Note that The file does not have to list attributes for every rigid body integrated by fix rigid. Only bodies which the file specifies will have their computed attributes overridden. The file can contain initial blank lines or comment lines starting with "#" which are ignored. The first non-blank,
non-comment line should list $N = \text{the number of lines to follow}$. The $N$ successive lines contain the following information:

```
ID1 masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz 
ID2 masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz 
... 
IDN masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz 
```

The rigid body IDs are all positive integers. For the single bodystyle, only an ID of 1 can be used. For the group bodystyle, IDs from 1 to $N_g$ can be used where $N_g$ is the number of specified groups. For the molecule bodystyle, use the molecule ID for the atoms in a specific rigid body as the rigid body ID.

The masstotal and center-of-mass coordinates ($xcm, ycm, zcm$) are self-explanatory. The center-of-mass should be consistent with what is calculated for the position of the rigid body with all its atoms unwrapped by their respective image flags. If this produces a center-of-mass that is outside the simulation box, LAMMPS wraps it back into the box. The 6 moments of inertia ($ixx, iyy, izz, ixy, ixz, iyz$) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the principal axes of the rigid body itself. LAMMPS performs the latter calculation internally.

**IMPORTANT NOTE:** The last point means that you cannot restart a simulation with rigid bodies using the `read_restart` command and use the same `infile` of rigid body attributes as input for the 2nd simulation, if the rigid bodies have moved or rotated. Instead, you need to produce a new `infile` that reflects the correct attributes for each rigid body at the time of restart. We are thinking about a good way to overcome this issue.

If you use a `temperature compute` with a group that includes particles in rigid bodies, the degrees-of-freedom removed by each rigid body are accounted for in the temperature (and pressure) computation, but only if the temperature group includes all the particles in a particular rigid body.

A 3d rigid body has 6 degrees of freedom (3 translational, 3 rotational), except for a collection of point particles lying on a straight line, which has only 5, e.g a dimer. A 2d rigid body has 3 degrees of freedom (2 translational, 1 rotational).

**IMPORTANT NOTE:** You may wish to explicitly subtract additional degrees-of-freedom if you use the `force` and `torque` keywords to eliminate certain motions of one or more rigid bodies. LAMMPS does not do this automatically.

The rigid body contribution to the pressure of the system (virial) is also accounted for by this fix.

**IMPORTANT NOTE:** The periodic image flags of atoms in rigid bodies are altered so that the rigid body can be reconstructed correctly when it straddles periodic boundaries. The atom image flags are not incremented/decremented as they would be for non-rigid atoms as the rigid body crosses periodic boundaries. This means you cannot interpret them as you normally would. For example, the image flag values written to a `dump file` will be different than they would be if the atoms were not in a rigid body. Likewise the `compute msd` will not compute the expected mean-squared displacement for such atoms if the body moves across periodic boundaries. It also means that if you have bonds between a pair of rigid bodies and the bond straddles a periodic boundary, you cannot use the `replicate` command to increase the system size. Note that this fix does define image flags for each rigid body, which are incremented when the rigid body crosses a periodic boundary in the usual way. These image flags have the same meaning as atom images (see the "dump" command) and can be accessed and output as described below.

**Restart, fix_modify, output, run start/stop, minimize info:**
No information about the rigid and rigid/nve fixes are written to binary restart files. For style rigid/nvt the state of the Nose/Hoover thermostat is written to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify energy option is supported by the rigid/nvt fix to add the energy change induced by the thermostating to the system's potential energy as part of thermodynamic output.

The fix_modify temp and press options are supported by the rigid/npt and rigid/nph fixes to change the computes used to calculate the instantaneous pressure tensor. Note that the rigid/nvt fix does not use any external compute to compute instantaneous temperature.

The rigid and rigid/nve fixes compute a global scalar which can be accessed by various output commands. The scalar value calculated by these fixes is "intensive". The scalar is the current temperature of the collection of rigid bodies. This is averaged over all rigid bodies and their translational and rotational degrees of freedom. The translational energy of a rigid body is 1/2 m v^2, where m = total mass of the body and v = the velocity of its center of mass. The rotational energy of a rigid body is 1/2 I w^2, where I = the moment of inertia tensor of the body and w = its angular velocity. Degrees of freedom constrained by the force and torque keywords are removed from this calculation.

The rigid/nvt, rigid/npt and rigid/nph fix compute a global scalar which can be accessed by various output commands. The scalar value calculated by these fixes is "extensive". The scalar is the cumulative energy change due to the thermostatting and barostatting the fix performs.

All of these fixes compute a global array of values which can be accessed by various output commands. The number of rows in the array is equal to the number of rigid bodies. The number of columns is 15. Thus for each rigid body, 15 values are stored: the xyz coords of the center of mass (COM), the xyz components of the COM velocity, the xyz components of the force acting on the COM, the xyz components of the torque acting on the COM, and the xyz image flags of the COM, which have the same meaning as image flags for atom positions (see the "dump" command). The force and torque values in the array are not affected by the force and torque keywords in the fix rigid command; they reflect values before any changes are made by those keywords.

The ordering of the rigid bodies (by row in the array) is as follows. For the single keyword there is just one rigid body. For the molecule keyword, the bodies are ordered by ascending molecule ID. For the group keyword, the list of group IDs determines the ordering of bodies.

The array values calculated by these fixes are "intensive", meaning they are independent of the number of atoms in the simulation.

No parameter of these fixes can be used with the start/stop keywords of the run command. These fixes are not invoked during energy minimization.

Restrictions:

These fixes performs an MPI_Allreduce each timestep that is proportional in length to the number of rigid bodies. Hence they will not scale well in parallel if large numbers of rigid bodies are simulated.

Related commands:

delete_bonds, neigh_modify exclude

Default:
The option defaults are force * on on on and torque * on on on, meaning all rigid bodies are acted on by center-of-mass force and torque. Also $T_{\text{chain}} = P_{\text{chain}} = 10$, $T_{\text{iter}} = 1$, $T_{\text{order}} = 3$.


fix setforce command

fix setforce/cuda command

Syntax:

fix ID group-ID setforce fx fy fz keyword value ...

- ID, group-ID are documented in fix command
- setforce = style name of this fix command
- fx,fy,fz = force component values
- any of fx,fy,fz can be a variable (see below)
- zero or more keyword/value pairs may be appended to args
- keyword = region

region value = region-ID
region-ID = ID of region atoms must be in to have added force

Examples:

fix freeze indenter setforce 0.0 0.0 0.0
fix 2 edge setforce NULL 0.0 0.0
fix 2 edge setforce NULL 0.0 v_oscillate

Description:

Set each component of force on each atom in the group to the specified values fx, fy, fz. This erases all previously computed forces on the atom, though additional fixes could add new forces. This command can be used to freeze certain atoms in the simulation by zeroing their force, either for running dynamics or performing an energy minimization. For dynamics, this assumes their initial velocity is also zero.

Any of the fx, fy, fz values can be specified as NULL which means do not alter the force component in that dimension.

Any of the 3 quantities defining the force components can be specified as an equal-style or atom-style variable, namely fx, fy, fz. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the force component.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent force field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent force field with optional time-dependence as well.

If the region keyword is used, the atom must also be in the specified geometric region in order to have force added to it.

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual.
The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix command-line switch` when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various output commands. This is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the `start/stop` keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command, but you cannot set forces to any value besides zero when performing a minimization. Use the fix addforce command if you want to apply a non-zero force to atoms during a minimization.

**Restrictions:** none

**Related commands:**

fix addforce, fix aveforce

**Default:** none
fix shake command

fix shake/cuda command

Syntax:

fix ID group-ID shake tol iter N keyword values ...

- ID, group-ID are documented in fix command
- shake = style name of this fix command
- tol = accuracy tolerance of SHAKE solution
- iter = max # of iterations in each SHAKE solution
- N = print SHAKE statistics every this many timesteps (0 = never)
- one or more keyword/value pairs are appended
- keyword = b or a or t or m

   b values = one or more bond types
   a values = one or more angle types
   t values = one or more atom types
   m value = one or more mass values

Examples:

fix 1 sub shake 0.0001 20 10 b 4 19 a 3 5 2
fix 1 sub shake 0.0001 20 10 t 5 6 m 1.0 a 31

Description:

Apply bond and angle constraints to specified bonds and angles in the simulation. This typically enables a longer timestep.

Each timestep the specified bonds and angles are reset to their equilibrium lengths and angular values via the well-known SHAKE algorithm. This is done by applying an additional constraint force so that the new positions preserve the desired atom separations. The equations for the additional force are solved via an iterative method that typically converges to an accurate solution in a few iterations. The desired tolerance (e.g. 1.0e-4 = 1 part in 10000) and maximum # of iterations are specified as arguments. Setting the N argument will print statistics to the screen and log file about regarding the lengths of bonds and angles that are being constrained. Small delta values mean SHAKE is doing a good job.

In LAMMPS, only small clusters of atoms can be constrained. This is so the constraint calculation for a cluster can be performed by a single processor, to enable good parallel performance. A cluster is defined as a central atom connected to others in the cluster by constrained bonds. LAMMPS allows for the following kinds of clusters to be constrained: one central atom bonded to 1 or 2 or 3 atoms, or one central atom bonded to 2 others and the angle between the 3 atoms also constrained. This means water molecules or CH2 or CH3 groups may be constrained, but not all the C-C backbone bonds of a long polymer chain.

The b keyword lists bond types that will be constrained. The t keyword lists atom types. All bonds connected to an atom of the specified type will be constrained. The m keyword lists atom masses. All bonds connected to atoms of the specified masses will be constrained (within a fudge factor of MASSDELTA specified in fix_shake.cpp). The a keyword lists angle types. If both bonds in the angle are constrained then the angle will also be constrained if its type is in the list.
For all keywords, a particular bond is only constrained if both atoms in the bond are in the group specified with the SHAKE fix.

The degrees-of-freedom removed by SHAKE bonds and angles are accounted for in temperature and pressure computations. Similarly, the SHAKE contribution to the pressure of the system (virial) is also accounted for.

IMPORTANT NOTE: This command works by using the current forces on atoms to calculate an additional constraint force which when added will leave the atoms in positions that satisfy the SHAKE constraints (e.g. bond length) after the next time integration step. If you define fixes (e.g. fix efield) that add additional force to the atoms after fix shake operates, then this fix will not take them into account and the time integration will typically not satisfy the SHAKE constraints. The solution for this is to make sure that fix shake is defined in your input script after any other fixes which add or change forces (to atoms that fix shake operates on).

Styles with a cuda suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

For computational efficiency, there can only be one shake fix defined in a simulation.

If you use a tolerance that is too large or a max-iteration count that is too small, the constraints will not be enforced very strongly, which can lead to poor energy conservation. You can test for this in your system by running a constant NVE simulation with a particular set of SHAKE parameters and monitoring the energy versus time.

Related commands: none

Default: none
fix smd command

Syntax:

fix ID group-ID smd type values keyword values

- ID, group-ID are documented in fix command
- smd = style name of this fix command
- mode = cvel or cfor to select constant velocity or constant force SMD

\[ \text{cvel values} = K \text{ vel} \]
\[ K = \text{spring constant (force/distance units)} \]
\[ \text{vel} = \text{velocity of pulling (distance/time units)} \]

\[ \text{cfor values} = \text{force} \]
\[ \text{force} = \text{pulling force (force units)} \]

- keyword = tether or couple

\[ \text{tether values} = x \ y \ z \ R0 \]
\[ x, y, z = \text{point to which spring is tethered} \]
\[ R0 = \text{distance of end of spring from tether point (distance units)} \]

\[ \text{couple values} = \text{group-ID2} \ x \ y \ z \ R0 \]
\[ \text{group-ID2} = \text{2nd group to couple to fix group with a spring} \]
\[ x, y, z = \text{direction of spring, automatically computed with 'auto'} \]
\[ R0 = \text{distance of end of spring (distance units)} \]

Examples:

fix pull cterm smd cvel 20.0 -0.00005 tether NULL NULL 100.0 0.0
fix pull cterm smd cvel 20.0 -0.0001 tether 25.0 25.0 25.0 0.0
fix stretch cterm smd cvel 20.0 0.0001 couple nterm auto auto auto 0.0
fix pull cterm smd cfor 5.0 tether 25.0 25.0 25.0 0.0

Description:

This fix implements several options of steered MD (SMD) as reviewed in (Izrailev), which allows to induce conformational changes in systems and to compute the potential of mean force (PMF) along the assumed reaction coordinate (Park) based on Jarzynski’s equality (Jarzynski). This fix borrows a lot from fix spring and fix setforce.

You can apply a moving spring force to a group of atoms (tether style) or between two groups of atoms (couple style). The spring can then be used in either constant velocity (cvel) mode or in constant force (cfor) mode to induce transitions in your systems. When running in tether style, you may need some way to fix some other part of the system (e.g. via fix spring/self)

The tether style attaches a spring between a point at a distance of R0 away from a fixed point x,y,z and the center of mass of the fix group of atoms. A restoring force of magnitude K (R - R0) Mi / M is applied to each atom in the group where K is the spring constant, Mi is the mass of the atom, and M is the total mass of all atoms in the group. Note that K thus represents the total force on the group of atoms, not a per-atom force.

In cvel mode the distance R is incremented or decremented monotonously according to the pulling (or pushing) velocity. In cfor mode a constant force is added and the actual distance in direction of the spring is recorded.

The couple style links two groups of atoms together. The first group is the fix group; the second is specified by group-ID2. The groups are coupled together by a spring that is at equilibrium when the two groups are displaced
by a vector in direction $x,y,z$ with respect to each other and at a distance $R_0$ from that displacement. Note that $x,y,z$ only provides a direction and will be internally normalized. But since it represents the absolute displacement of group-ID2 relative to the fix group, $(1,1,0)$ is a different spring than $(-1,-1,0)$. For each vector component, the displacement can be described with the auto parameter. In this case the direction is recomputed in every step, which can be useful for steering a local process where the whole object undergoes some other change. When the relative positions and distance between the two groups are not in equilibrium, the same spring force described above is applied to atoms in each of the two groups.

For both the tether and couple styles, any of the $x,y,z$ values can be specified as NULL which means do not include that dimension in the distance calculation or force application.

For constant velocity pulling (cvel mode), the running integral over the pulling force in direction of the spring is recorded and can then later be used to compute the potential of mean force (PMF) by averaging over multiple independent trajectories along the same pulling path.

**Restart, fix_modify, output, run start/stop, minimize info:**

The fix stores the direction of the spring, current pulling target distance and the running PMF to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix.

This fix computes a vector list of 7 quantities, which can be accessed by various output commands. The quantities in the vector are in this order: the $x$-, $y$-, and $z$-component of the pulling force, the total force in direction of the pull, the equilibrium distance of the spring, the distance between the two reference points, and finally the accumulated PMF (the sum of pulling forces times displacement).

The force is the total force on the group of atoms by the spring. In the case of the couple style, it is the force on the fix group (group-ID) or the negative of the force on the 2nd group (group-ID2). The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

fix drag, fix spring, fix spring/self, fix spring/rg

**Default:**

none


fix spring command

Syntax:

fix ID group-ID spring keyword values

- ID, group-ID are documented in fix command
- spring = style name of this fix command
- keyword = tether or couple

tether values = \( K \times x \times y \times z \times R_0 \)
- \( K \) = spring constant (force/distance units)
- \( x, y, z \) = point to which spring is tethered
- \( R_0 \) = equilibrium distance from tether point (distance units)

couple values = group-ID2 \( K \times x \times y \times z \times R_0 \)
- group-ID2 = 2nd group to couple to fix group with a spring
- \( K \) = spring constant (force/distance units)
- \( x, y, z \) = direction of spring
- \( R_0 \) = equilibrium distance of spring (distance units)

Examples:

fix pull ligand spring tether 50.0 0.0 0.0 0.0 0.0
fix pull ligand spring tether 50.0 0.0 0.0 0.0 5.0
fix pull ligand spring tether 50.0 NULL NULL 2.0 3.0
fix 5 bilayer1 spring couple bilayer2 100.0 NULL NULL 10.0 0.0
fix longitudinal pore spring couple ion 100.0 NULL NULL -20.0 0.0
fix radial pore spring couple ion 100.0 0.0 0.0 NULL 5.0

Description:

Apply a spring force to a group of atoms or between two groups of atoms. This is useful for applying an umbrella force to a small molecule or lightly tethering a large group of atoms (e.g. all the solvent or a large molecule) to the center of the simulation box so that it doesn't wander away over the course of a long simulation. It can also be used to hold the centers of mass of two groups of atoms at a given distance or orientation with respect to each other.

The *tether* style attaches a spring between a fixed point \( x, y, z \) and the center of mass of the fix group of atoms. The equilibrium position of the spring is \( R_0 \). At each timestep the distance \( R \) from the center of mass of the group of atoms to the tethering point is computed, taking account of wrap-around in a periodic simulation box. A restoring force of magnitude \( K (R - R_0) M_i / M \) is applied to each atom in the group where \( K \) is the spring constant, \( M_i \) is the mass of the atom, and \( M \) is the total mass of all atoms in the group. Note that \( K \) thus represents the total force on the group of atoms, not a per-atom force.

The *couple* style links two groups of atoms together. The first group is the fix group; the second is specified by group-ID2. The groups are coupled together by a spring that is at equilibrium when the two groups are displaced by a vector \( x, y, z \) with respect to each other and at a distance \( R_0 \) from that displacement. Note that \( x, y, z \) is the equilibrium displacement of group-ID2 relative to the fix group. Thus \((1,1,0)\) is a different spring than \((-1,-1,0)\). When the relative positions and distance between the two groups are not in equilibrium, the same spring force described above is applied to atoms in each of the two groups.

For both the *tether* and *couple* styles, any of the \( x, y, z \) values can be specified as NULL which means do not include that dimension in the distance calculation or force application.
The first example above pulls the ligand towards the point (0,0,0). The second example holds the ligand near the surface of a sphere of radius 5 around the point (0,0,0). The third example holds the ligand a distance 3 away from the z=2 plane (on either side).

The fourth example holds 2 bilayers a distance 10 apart in z. For the last two examples, imagine a pore (a slab of atoms with a cylindrical hole cut out) oriented with the pore axis along z, and an ion moving within the pore. The fifth example holds the ion a distance of -20 below the z = 0 center plane of the pore (umbrella sampling). The last example holds the ion a distance 5 away from the pore axis (assuming the center-of-mass of the pore in x,y is the pore axis).

IMPORTANT NOTE: The center of mass of a group of atoms is calculated in "unwrapped" coordinates using atom image flags, which means that the group can straddle a periodic boundary. See the dump doc page for a discussion of unwrapped coordinates. It also means that a spring connecting two groups or a group and the tether point can cross a periodic boundary and its length be calculated correctly. One exception is for rigid bodies, which should not be used with the fix spring command, if the rigid body will cross a periodic boundary. This is because image flags for rigid bodies are used in a different way, as explained on the fix rigid doc page.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify energy option is supported by this fix to add the energy stored in the spring to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the spring energy = 0.5 * K * r^2.

This fix also computes global 4-vector which can be accessed by various output commands. The first 3 quantities in the vector are xyz components of the total force added to the group of atoms by the spring. In the case of the couple style, it is the force on the fix group (group-ID) or the negative of the force on the 2nd group (group-ID2). The 4th quantity in the vector is the magnitude of the force added by the spring, as a positive value if (r-R0) > 0 and a negative value if (r-R0) < 0. This sign convention can be useful when using the spring force to compute a potential of mean force (PMF).

The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

IMPORTANT NOTE: If you want the spring energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify energy option for this fix.

Restrictions: none

Related commands:

fix drag, fix spring/self, fix spring/rg, fix smd

Default: none
fix spring/rg command

Syntax:

fix ID group-ID spring/rg K RG0

- ID, group-ID are documented in fix command
- spring/rg = style name of this fix command
- K = harmonic force constant (force/distance units)
- RG0 = target radius of gyration to constrain to (distance units)

if RG0 = NULL, use the current RG as the target value

Examples:

fix 1 protein spring/rg 5.0 10.0
fix 2 micelle spring/rg 5.0 NULL

Description:

Apply a harmonic restraining force to atoms in the group to affect their central moment about the center of mass (radius of gyration). This fix is useful to encourage a protein or polymer to fold/unfold and also when sampling along the radius of gyration as a reaction coordinate (i.e. for protein folding).

The radius of gyration is defined as RG in the first formula. The energy of the constraint and associated force on each atom is given by the second and third formulas, when the group is at a different RG than the target value RG0.

\[ R_G^2 = \frac{1}{M} \sum_{i}^{N} m_i \left( x_i - \frac{1}{M} \sum_{j}^{N} m_j x_j \right)^2 \]

\[ E = K \left( R_G - R_{G0} \right)^2 \]

\[ F_i = 2K \frac{m_i}{M} \left( 1 - \frac{R_{G0}}{R_G} \right) \left( x_i - \frac{1}{M} \sum_{j}^{N} m_j x_j \right) \]

The \((x_i - \text{center-of-mass})\) term is computed taking into account periodic boundary conditions, \(m_i\) is the mass of the atom, and \(M\) is the mass of the entire group. Note that \(K\) is thus a force constant for the aggregate force on the group of atoms, not a per-atom force.

If RG0 is specified as NULL, then the RG of the group is computed at the time the fix is specified, and that value is used as the target.
**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

fix spring, fix spring/self fix drag, fix smd

**Default:** none
**fix spring/self command**

**Syntax:**

```plaintext
fix ID group-ID spring/self K dir
```

- ID, group-ID are documented in fix command
- spring/self = style name of this fix command
- K = spring constant (force/distance units)
- dir = xyz, xy, xz, yz, x, y, or z (optional, default: xyz)

**Examples:**

```plaintext
fix tether boundary-atoms spring/self 10.0
fix zrest move spring/self 10.0 z
```

**Description:**

Apply a spring force independently to each atom in the group to tether it to its initial position. The initial position for each atom is its location at the time the fix command was issued. At each timestep, the magnitude of the force on each atom is -Kr, where r is the displacement of the atom from its current position to its initial position.

With the (optional) dir flag, one can select in which direction the spring force is applied. By default, the restraint is applied in all directions, but it can be limited to the xy-, xz-, yz-plane and the x-, y-, or z-direction, thus restraining the atoms to a line or a plane, respectively.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the original coordinates of tethered atoms to binary restart files, so that the spring effect will be the same in a restarted simulation. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify energy option is supported by this fix to add the energy stored in the per-atom springs to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is an energy which is the sum of the spring energy for each atom, where the per-atom energy is 0.5 * K * r^2. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

**IMPORTANT NOTE:** If you want the per-atom spring energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify energy option for this fix.

**Restrictions:** none

**Related commands:**
fix drag, fix spring, fix smd, fix spring/rg

Default: none
fix srd command

Syntax:

```
fix ID group-ID srd N groupbig-ID Tsrd hgrid seed keyword value ...
```

- ID, group-ID are documented in fix command
- srd = style name of this fix command
- N = reset SRD particle velocities every this many timesteps
- groupbig-ID = ID of group of large particles that SRDs interact with
- Tsrd = temperature of SRD particles (temperature units)
- hgrid = grid spacing for SRD grouping (distance units)
- seed = random # seed (positive integer)
- zero or more keyword/value pairs may be appended
- keyword = lamda or collision or overlap or inside or exact or radius or bounce or search or cubic or shift or stream

- lamda value = mean free path of SRD particles (distance units)
- collision value = noslip or slip = collision model
- overlap value = yes or no = whether big particles may overlap
- inside value = error or warn or ignore = how SRD particles which end up inside a big particle are treated
- exact value = yes or no
- radius value = rfactor = scale collision radius by this factor
- bounce value = Nbounce = max # of collisions an SRD particle can undergo in one timestep
- search value = sgrid = grid spacing for collision partner searching (distance units)
- cubic values = style tolerance
  - style = error or warn
  - tolerance = fractional difference allowed (0 <= tol <= 1)
- tstat value = yes or no = thermostat SRD particles or not

Examples:

```
fix 1 srd srd 10 big 1.0 0.25 482984
fix 1 srd srd 10 big 0.5 0.25 482984 collision slip search 0.5
```

Description:

Treat a group of particles as stochastic rotation dynamics (SRD) particles that serve as a background solvent when interacting with big (colloidal) particles in groupbig-ID. The SRD formalism is described in (Hecht). The key idea behind using SRD particles as a cheap coarse-grained solvent is that SRD particles do not interact with each other, but only with the solute particles, which in LAMMPS can be spheroids, ellipsoids, or line segments, or triangles, or rigid bodies containing multiple spheroids or ellipsoids or line segments or triangles. The collision and rotation properties of the model imbue the SRD particles with fluid-like properties, including an effective viscosity. Thus simulations with large solute particles can be run more quickly, to measure solute properties like diffusivity and viscosity in a background fluid. The usual LAMMPS fixes for such simulations, such as fix deform, fix viscosity, and fix nvt/sllod, can be used in conjunction with the SRD model.

For more details on how the SRD model is implemented in LAMMPS, this paper describes the implementation and usage of pure SRD fluids. This paper, which is nearly complete, describes the implementation and usage of mixture systems (solute particles in an SRD fluid). See the examples/srd directory for sample input scripts using SRD particles in both settings.
This fix does 2 things:

(1) It advects the SRD particles, performing collisions between SRD and big particles or walls every timestep, imparting force and torque to the big particles. Collisions also change the position and velocity of SRD particles.

(2) It resets the velocity distribution of SRD particles via random rotations every N timesteps.

SRD particles have a mass, temperature, characteristic timestep $dt_{SRD}$, and mean free path between collisions ($\lambda$). The fundamental equation relating these 4 quantities is

$$\lambda = dt_{SRD} \times \sqrt{K_{boltz} \times Tsrd / mass}$$

The mass of SRD particles is set by the mass command elsewhere in the input script. The SRD timestep $dt_{SRD}$ is N times the step $dt$ defined by the timestep command. Big particles move in the normal way via a time integration fix with a short timestep $dt$. SRD particles advect with a large timestep $dt_{SRD} \geq dt$.

If the $\lambda$ keyword is not specified, the the SRD temperature $Tsrd$ is used in the above formula to compute $\lambda$. If the $\lambda$ keyword is specified, then the $Tsrd$ setting is ignored and the above equation is used to compute the SRD temperature.

The characteristic length scale for the SRD fluid is set by $hgrid$ which is used to bin SRD particles for purposes of resetting their velocities. Normally $hgrid$ is set to be 1/4 of the big particle diameter or smaller, to adequately resolve fluid properties around the big particles.

$\lambda$ cannot be smaller than $0.6 \times hgrid$, else an error is generated (unless the shift keyword is used, see below). The velocities of SRD particles are bounded by $Vmax$, which is set so that an SRD particle will not advect further than $Dmax = 4 \times \lambda$ in $dt_{SRD}$. This means that roughly speaking, $Dmax$ should not be larger than a big particle diameter, else SRDs may pass thru big particles without colliding. A warning is generated if this is the case.

Collisions between SRD particles and big particles or walls are modeled as a lightweight SRD point particle hitting a heavy big particle of given diameter or a wall at a point on its surface and bouncing off with a new velocity. The collision changes the momentum of the SRD particle. It imparts a force and torque to the big particle. It imparts a force to a wall. Static or moving SRD walls are setup via the fix wall/srd command. For the remainder of this doc page, a collision of an SRD particle with a wall can be viewed as a collision with a big particle of infinite radius and mass.

The collision keyword sets the style of collisions. The slip style means that the tangential component of the SRD particle momentum is preserved. Thus a force is imparted to a big particle, but no torque. The normal component of the new SRD velocity is sampled from a Gaussian distribution at temperature $Tsrd$.

For the noslip style, both the normal and tangential components of the new SRD velocity are sampled from a Gaussian distribution at temperature $Tsrd$. Additionally, a new tangential direction for the SRD velocity is chosen randomly. This collision style imparts torque to a big particle. Thus a time integrator fix that rotates the big particles appropriately should be used.

The overlap keyword should be set to yes if two (or more) big particles can ever overlap. This depends on the pair potential interaction used for big-big interactions, or could be the case if multiple big particles are held together as rigid bodies via the fix rigid command. If the overlap keyword is no and big particles do in fact overlap, then SRD/big collisions can generate an error if an SRD ends up inside two (or more) big particles at once. How this error is treated is determined by the inside keyword. Running with overlap set to no allows for faster collision checking, so it should only be set to yes if needed.
The *inside* keyword determines how a collision is treated if the computation determines that the timestep started with the SRD particle already inside a big particle. If the setting is *error* then this generates an error message and LAMMPS stops. If the setting is *warn* then this generates a warning message and the code continues. If the setting is *ignore* then no message is generated. One of the output quantities logged by the fix (see below) tallies the number of such events, so it can be monitored. Note that once an SRD particle is inside a big particle, it may remain there for several steps until it drifts outside the big particle.

The *exact* keyword determines how accurately collisions are computed. A setting of *yes* computes the time and position of each collision as SRD and big particles move together. A setting of *no* estimates the position of each collision based on the end-of-timestep positions of the SRD and big particle. If *overlap* is set to *yes*, the setting of the *exact* keyword is ignored since time-accurate collisions are needed.

The *radius* keyword scales the effective size of big particles. If big particles will overlap as they undergo dynamics, then this keyword can be used to scale down their effective collision radius by an amount *rfactor*, so that SRD particle will only collide with one big particle at a time. For example, in a Lennard-Jones system at a temperature of 1.0 (in reduced LJ units), the minimum separation between two big particles is as small as about 0.88 sigma. Thus an *rfactor* value of 0.85 should prevent dual collisions.

The *bounce* keyword can be used to limit the maximum number of collisions an SRD particle undergoes in a single timestep as it bounces between nearby big particles. Note that if the limit is reached, the SRD can be left inside a big particle. A setting of 0 is the same as no limit.

There are 2 kinds of bins created and maintained when running an SRD simulation. The first are "SRD bins" which are used to bin SRD particles and reset their velocities, as discussed above. The second are "search bins" which are used to identify SRD/big particle collisions.

The *search* keyword can be used to choose a search bin size for identifying SRD/big particle collisions. The default is to use the *hgrid* parameter for SRD bins as the search bin size. Choosing a smaller or large value may be more efficient, depending on the problem. But, in a statistical sense, it should not change the simulation results.

The *cubic* keyword can be used to generate an error or warning when the bin size chosen by LAMMPS creates SRD bins that are non-cubic or different than the requested value of *hgrid* by a specified *tolerance*. Note that using non-cubic SRD bins can lead to undetermined behavior when rotating the velocities of SRD particles, hence LAMMPS tries to protect you from this problem.

LAMMPS attempts to set the SRD bin size to exactly *hgrid*. However, there must be an integer number of bins in each dimension of the simulation box. Thus the actual bin size will depend on the size and shape of the overall simulation box. The actual bin size is printed as part of the SRD output when a simulation begins.

If the actual bin size in non-cubic by an amount exceeding the tolerance, an error or warning is printed, depending on the style of the *cubic* keyword. Likewise, if the actual bin size differs from the requested *hgrid* value by an amount exceeding the tolerance, then an error or warning is printed. The *tolerance* is a fractional difference. E.g. a tolerance setting of 0.01 on the shape means that if the ratio of any 2 bin dimensions exceeds (1 +/- tolerance) then an error or warning is generated. Similarly, if the ratio of any bin dimension with *hgrid* exceeds (1 +/- tolerance), then an error or warning is generated.

IMPORTANT NOTE: The fix srd command can be used with simulations the size and/or shape of the simulation box changes. This can be due to non-periodic boundary conditions or the use of fixes such as the fix deform or fix wall/srd commands to impose a shear on an SRD fluid or an interaction with an external wall. If the box size changes then the size of SRD bins must be recalculated every reneighboring. This is not necessary if only the box shape changes. This re-binning is always done so as to fit an integer number of bins in the current box dimension, whether it be a fixed, shrink-wrapped, or periodic boundary, as set by the *boundary* command. If the box size or
shape changes, then the size of the search bins must be recalculated every reneighboring. Note that changing the SRD bin size may alter the properties of the SRD fluid, such as its viscosity.

The \textit{shift} keyword determines whether the coordinates of SRD particles are randomly shifted when binned for purposes of rotating their velocities. When no shifting is performed, SRD particles are binned and the velocity distribution of the set of SRD particles in each bin is adjusted via a rotation operator. This is a statistically valid operation if SRD particles move sufficiently far between successive rotations. This is determined by their mean-free path \(\lambda\). If \(\lambda\) is less than 0.6 of the SRD bin size, then shifting is required. A shift means that all of the SRD particles are shifted by a vector whose coordinates are chosen randomly in the range \([-1/2 \text{ bin size}, 1/2 \text{ bin size}]\). Note that all particles are shifted by the same vector. The specified random number seed is used to generate these vectors. This operation sufficiently randomizes which SRD particles are in the same bin, even if \(\lambda\) is small.

If the \textit{shift} style is set to \textit{no}, then no shifting is performed, but bin data will be communicated if bins overlap processor boundaries. An error will be generated if \(\lambda < 0.6\) of the SRD bin size. If the \textit{shift} style is set to \textit{possible}, then shifting is performed only if \(\lambda < 0.6\) of the SRD bin size. A warning is generated to let you know this is occurring. If the \textit{shift} style is set to \textit{yes} then shifting is performed regardless of the magnitude of \(\lambda\).

The shift seed is not used if the \textit{shift} style is set to \textit{no}, but must still be specified.

Note that shifting of SRD coordinates requires extra communication, hence it should not normally be enabled unless required.

The \textit{tstat} keyword will thermostat the SRD particles to the specified \(T_{srd}\). This is done every N timesteps, during the velocity rotation operation, by rescaling the thermal velocity of particles in each SRD bin to the desired temperature. If there is a streaming velocity associated with the system, e.g. due to use of the fix deform command to perform a simulation undergoing shear, then that is also accounted for. The mean velocity of each bin of SRD particles is set to the position-dependent streaming velocity, based on the coordinates of the center of the SRD bin. Note that for streaming simulations, if no thermostatting is performed (the default), then it may take a long time for the SRD fluid to come to equilibrium with a velocity profile that matches the simulation box deformation.

\textbf{IMPORTANT NOTE:} This fix is normally used for simulations with a huge number of SRD particles relative to the number of big particles, e.g. 100 to 1. In this scenario, computations that involve only big particles (neighbor list creation, communication, time integration) can slow down dramatically due to the large number of background SRD particles.

Three other input script commands will largely overcome this effect, speeding up an SRD simulation by a significant amount. These are the \texttt{atom_modify first}, \texttt{neigh_modify include}, and \texttt{communicate group} commands. Each takes a group-ID as an argument, which in this case should be the group-ID of the big solute particles.

Additionally, when a pair style for big/big particle interactions is specified, the \texttt{pair_coeff} command should be used to turn off big/SRD interactions, e.g. by setting their epsilon or cutoff length to 0.0.

The "delete_atoms overlap" command may be useful in setting up an SRD simulation to insure there are no initial overlaps between big and SRD particles.

\textbf{Restart, fix_modify, output, run start/stop, minimize info:}

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.
This fix tabulates several SRD statistics which are stored in a vector of length 12, which can be accessed by various output commands. The vector values calculated by this fix are "intensive", meaning they do not scale with the size of the simulation. Technically, the first 8 do scale with the size of the simulation, but treating them as intensive means they are not scaled when printed as part of thermodynamic output.

These are the 12 quantities. All are values for the current timestep, except the last three which are cumulative quantities since the beginning of the run.

- (1) # of SRD/big collision checks performed
- (2) # of SRDs which had a collision
- (3) # of SRD/big collisions (including multiple bounces)
- (4) # of SRD particles inside a big particle
- (5) # of SRD particles whose velocity was rescaled to be < Vmax
- (6) # of bins for collision searching
- (7) # of bins for SRD velocity rotation
- (8) # of bins in which SRD temperature was computed
- (9) SRD temperature
- (10) # of SRD particles which have undergone max # of bounces
- (11) max # of bounces any SRD particle has had in a single step
- (12) # of reneighborings due to SRD particles moving too far

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This command can only be used if LAMMPS was built with the SRD package. See the Making LAMMPS section for more info on packages.

Related commands:

fix wall/srd

Default:

The option defaults are lamda inferred from Tsrd, collision = noslip, overlap = no, inside = error, exact = yes, radius = 1.0, bounce = 0, search = hgrid, cubic = error 0.01, shift = no, tstat = no.

(Hecht) Hecht, Harting, Ihle, Herrmann, Phys Rev E, 72, 011408 (2005).


**fix store/force command**

**Syntax:**

```plaintext
fix ID group-ID store/force
```

- ID, group-ID are documented in fix command
- store/force = style name of this fix command

**Examples:**

```plaintext
fix 1 all store/force
```

**Description:**

Store the forces on atoms in the group at the point during each timestep when the fix is invoked, as described below. This is useful for storing forces before constraints or other boundary conditions are computed which modify the forces, so that unmodified forces can be written to a dump file or accessed by other output commands that use per-atom quantities.

This fix is invoked at the point in the velocity-Verlet timestepping immediately after pair, bond, angle, dihedral, improper, and long-range forces have been calculated. It is the point in the timestep when various fixes that compute constraint forces are calculated and potentially modify the force on each atom. Examples of such fixes are fix shake, fix wall, and fix indent.

IMPORTANT NOTE: The order in which various fixes are applied which operate at the same point during the timestep, is the same as the order they are specified in the input script. Thus normally, if you want to store per-atom forces due to force field interactions, before constraints are applied, you should list this fix first within that set of fixes, i.e. before other fixes that apply constraints. However, if you wish to include certain constraints (e.g. fix shake) in the stored force, then it could be specified after some fixes and before others.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix produces a per-atom array which can be accessed by various output commands. The number of columns for each atom is 3, and the columns store the x,y,z forces on each atom. The per-atom values be accessed on any timestep.

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

fix store_state

**Default:** none
**fix store/state command**

**Syntax:**

```
fix ID group-ID store/state N input1 input2 ... keyword value ...
```

- ID, group-ID are documented in fix command
- store/state = style name of this fix command
- N = store atom attributes every N steps, N = 0 for initial store only
- input = one or more atom attributes

possible attributes = id, mol, type, mass,
  x, y, z, xs, ys, zs, xu, yu, zu, ix, iy, iz,
  vx, vy, vz, fx, fy, fz,
  q, mux, muy, muz,
  radius, omegax, omegay, omegaz,
  angmomx, angmomy, angmomz, tqx, tqy, tqz
  c_ID, c_ID[N], f_ID, f_ID[N], v_name

- id = atom ID
- mol = molecule ID
- type = atom type
- mass = atom mass
- x, y, z = unscaled atom coordinates
- xs, ys, zs = scaled atom coordinates
- xu, yu, zu = unwrapped atom coordinates
- ix, iy, iz = box image that the atom is in
- vx, vy, vz = atom velocities
- fx, fy, fz = forces on atoms
- q = atom charge
- mux, muy, muz = orientation of dipolar atom
- radius = radius of extended spherical particle
- omegax, omegay, omegaz = angular velocity of extended particle
- angmomx, angmomy, angmomz = angular momentum of extended particle
- tqx, tqy, tqz = torque on extended particles
- c_ID = per-atom vector calculated by a compute with ID
- c_ID[N] = Ith column of per-atom array calculated by a compute with ID
- f_ID = per-atom vector calculated by a fix with ID
- f_ID[N] = Ith column of per-atom array calculated by a fix with ID
- v_name = per-atom vector calculated by an atom-style variable with name

- zero or more keyword/value pairs may be appended
- keyword = com

```
com value = yes or no
```

**Examples:**

```
fix 1 all store/state 0 x y z
fix 1 all store/state 0 xu yu zu com yes
fix 2 all store/state 1000 vx vy vz
```

**Description:**

Define a fix that stores attributes for each atom in the group at the time the fix is defined. If $N$ is 0, then the values are never updated, so this is a way of archiving an atom attribute at a given time for future use in a calculation or output. See the discussion of output commands that take fixes as inputs. And see for example, the compute
reduce, fix ave/atom, fix ave/histo, fix ave/spatial, and atom-style variable commands.

If $N$ is not zero, then the attributes will be updated every $N$ steps.

IMPORTANT NOTE: Actually, only atom attributes specified by keywords like $xu$ or $vy$ are initially stored immediately at the point in your input script when the fix is defined. Attributes specified by a compute, fix, or variable are not initially stored until the first run following the fix definition begins. This is because calculating those attributes may require quantities that are not defined in between runs.

The list of possible attributes is the same as that used by the dump custom command, which describes their meaning.

If the com keyword is set to yes then the $xu$, $yu$, and $zu$ inputs store the position of each atom relative to the center-of-mass of the group of atoms, instead of storing the absolute position. This option is used by the compute msd command.

The requested values are stored in a per-atom vector or array as discussed below. Zeroes are stored for atoms not in the specified group.

**Restart, fix_modify, output, run start/stop, minimize info:**

This fix writes the per-atom values it stores to binary restart files, so that the values can be restored when a simulation is restarted. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix.

If a single input is specified, this fix produces a per-atom vector. If multiple inputs are specified, a per-atom array is produced where the number of columns for each atom is the number of inputs. These can be accessed by various output commands. The per-atom values be accessed on any timestep.

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:** none

**Related commands:**

dump custom, compute property/atom, variable

**Default:**

The option default is com = no.
fix temp/berendsen command

fix temp/berendsen/cuda command

Syntax:

fix ID group-ID temp/berendsen Tstart Tstop Tdamp

- ID, group-ID are documented in fix command
- temp/berendsen = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run
- Tdamp can be a variable (see below)
- Tdamp = temperature damping parameter (time units)

Examples:

fix 1 all temp/berendsen 300.0 300.0 100.0

Description:

Reset the temperature of a group of atoms by using a Berendsen thermostat (Berendsen), which rescales their velocities every timestep.

The thermostat is applied to only the translational degrees of freedom for the particles, which is an important consideration if extended spherical or aspherical particles which have rotational degrees of freedom are being thermostatted with this fix. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

The desired temperature at each timestep is a ramped value during the run from Tstart to Tstop. The Tdamp parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the units command).

Tstart can be specified as an equal-style variable. In this case, the Tstop setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

IMPORTANT NOTE: Unlike the fix nvt command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies velocities to effect thermostatting. Thus you must use a separate time integration fix, like fix nve to actually update the positions of atoms using the modified velocities. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by fix nvt or fix langevin commands.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.
This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp", as if this command had been issued:

```plaintext
compute fix-ID_temp group-ID temp
```

See the `compute temp` command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the `thermo_style` command) with ID = `thermo_temp`. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the `compute_modify` command or print this temperature during thermodynamic output via the `thermo_style custom` command using the appropriate compute-ID. It also means that changing attributes of `thermo_temp` will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with `compute commands` that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the `fix_modify` command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual `compute commands` to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a `cuda` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in `Section_accelerate` of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the `Making LAMMPS` section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See `Section_accelerate` of the manual for more instructions on how to use the accelerated styles effectively.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files.

The `fix_modify temp` option is supported by this fix. You can use it to assign a temperature `compute` you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The `fix_modify energy` option is supported by this fix to add the energy change implied by a velocity rescaling to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various `output commands`. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".
This fix can ramp its target temperature over multiple runs, using the \textit{start} and \textit{stop} keywords of the \texttt{run} command. See the \texttt{run} command for details of how to do this.

This fix is not invoked during \textit{energy minimization}.

\textbf{Restrictions:} none

\textbf{Related commands:}

\texttt{fix nve, fix nvt, fix temp/rescale, fix langevin, fix\_modify, compute temp, fix press/berendsen}

\textbf{Default:} none

**fix temp/rescale command**

**fix temp/rescale/cuda command**

**fix temp/rescale/limit/cuda command**

**Syntax:**

```
fix ID group-ID temp/rescale N Tstart Tstop window fraction
```

- ID, group-ID are documented in fix command
- temp/rescale = style name of this fix command
- N = perform rescaling every N steps
- Tstart, Tstop = desired temperature at start/end of run (temperature units)

  Tstart can be a variable (see below)

- window = only rescale if temperature is outside this window (temperature units)
- fraction = rescale to target temperature by this fraction

**Examples:**

```
fix 3 flow temp/rescale 100 1.0 1.1 0.02 0.5
fix 3 boundary temp/rescale 1 1.0 1.5 0.05 1.0
fix 3 boundary temp/rescale 1 1.0 1.5 0.05 1.0
```

**Description:**

Reset the temperature of a group of atoms by explicitly rescaling their velocities.

The rescaling is applied to only the translational degrees of freedom for the particles, which is an important consideration if extended spherical or aspherical particles which have rotational degrees of freedom are being thermostatted with this fix. The translational degrees of freedom can also have a bias velocity removed from them before thermostating takes place; see the description below.

Rescaling is performed every N timesteps. The target temperature is a ramped value between the \( T_{\text{start}} \) and \( T_{\text{stop}} \) temperatures at the beginning and end of the run.

\( T_{\text{start}} \) can be specified as an equal-style variable. In this case, the \( T_{\text{stop}} \) setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Rescaling is only performed if the difference between the current and desired temperatures is greater than the window value. The amount of rescaling that is applied is a fraction (from 0.0 to 1.0) of the difference between the actual and desired temperature. E.g. if fraction = 1.0, the temperature is reset to exactly the desired value.
IMPORTANT NOTE: Unlike the `fix nvt` command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies velocities to effect thermostatting. Thus you must use a separate time integration fix, like `fix nve` to actually update the positions of atoms using the modified velocities. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by `fix nvt` or `fix langevin` commands.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp", as if one of this command had been issued:

```
compute fix-ID_temp group-ID temp
```

See the `compute temp` for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the `thermo_style` command) with ID = `thermo_temp`. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the `compute_modify` command or print this temperature during thermodynamic output via the `thermo_style custom` command using the appropriate compute-ID. It also means that changing attributes of `thermo_temp` will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with `compute commands` that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the `fix_modify` command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual `compute commands` to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a `cuda` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files.

The `fix_modify temp` option is supported by this fix. You can use it to assign a temperature `compute` you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the
group used by this fix and by the compute should be the same.

The fix_modify energy option is supported by this fix to add the energy change implied by a velocity rescaling to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix can ramp its target temperature over multiple runs, using the start and stop keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix langevin, fix nvt, fix_modify

Default: none
**fix temp/rescale/eff command**

**Syntax:**

```plaintext
fix ID group-ID temp/rescale/eff N Tstart Tstop window fraction
```

- ID, group-ID are documented in **fix** command
- temp/rescale/eff = style name of this fix command
- N = perform rescaling every N steps
- Tstart, Tstop = desired temperature at start/end of run (temperature units)
- window = only rescale if temperature is outside this window (temperature units)
- fraction = rescale to target temperature by this fraction

**Examples:**

```plaintext
fix 3 flow temp/rescale/eff 10 1.0 100.0 0.02 1.0
```

**Description:**

Reset the temperature of a group of nuclei and electrons in the electron force field model by explicitly rescaling their velocities.

The operation of this fix is exactly like that described by the **fix temp/rescale** command, except that the rescaling is also applied to the radial electron velocity for electron particles.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files.

The **fix_modify temp** option is supported by this fix. You can use it to assign a temperature **compute** you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The **fix_modify energy** option is supported by this fix to add the energy change implied by a velocity rescaling to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various **output commands**. The scalar is the cumulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix can ramp its target temperature over multiple runs, using the **start** and **stop** keywords of the **run** command. See the **run** command for details of how to do this.

This fix is not invoked during **energy minimization**.

**Restrictions:**

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the **Making LAMMPS** section for more info.

**Related commands:**
fix langevin/eff, fix nvt/eff, fix_modify, fix_temp_rescale,

**Default:** none
fix thermal/conductivity command

Syntax:

fix ID group-ID thermal/conductivity N edim Nbin keyword value ...

- ID, group-ID are documented in fix command
- thermal/conductivity = style name of this fix command
- N = perform kinetic energy exchange every N steps
- edim = x or y or z = direction of kinetic energy transfer
- Nbin = # of layers in edim direction (must be even number)
- zero or more keyword/value pairs may be appended
- keyword = swap

  swap value = Nswap = number of swaps to perform every N steps

Examples:

fix 1 all thermal/conductivity 100 z 20
fix 1 all thermal/conductivity 50 z 20 swap 2

Description:

Use the Muller-Plathe algorithm described in this paper to exchange kinetic energy between two particles in different regions of the simulation box every N steps. This induces a temperature gradient in the system. As described below this enables a thermal conductivity of the fluid to be calculated. This algorithm is sometimes called a reverse non-equilibrium MD (reverse NEMD) approach to computing thermal conductivity. This is because the usual NEMD approach is to impose a temperature gradient on the system and measure the response as the resulting heat flux. In the Muller-Plathe method, the heat flux is imposed, and the temperature gradient is the system's response.

See the compute heat/flux command for details on how to compute thermal conductivity in an alternate way, via the Green-Kubo formalism.

The simulation box is divided into Nbin layers in the edim direction, where the layer 1 is at the low end of that dimension and the layer Nbin is at the high end. Every N steps, Nswap pairs of atoms are chosen in the following manner. Only atoms in the fix group are considered. The hottest Nswap atoms in layer 1 are selected. Similarly, the coldest Nswap atoms in the "middle" layer (see below) are selected. The two sets of Nswap atoms are paired up and their velocities are exchanged. This effectively swaps their kinetic energies, assuming their masses are the same. Over time, this induces a temperature gradient in the system which can be measured using commands such as the following, which writes the temperature profile (assuming z = edim) to the file tmp.profile:

```
compute   ke all ke/atom
variable  temp atom c_ke/1.5
fix       3 all ave/spatial 10 100 1000 z lower 0.05 v_temp &
          file tmp.profile units reduced
```

Note that by default, Nswap = 1, though this can be changed by the optional swap keyword. Setting this parameter appropriately, in conjunction with the swap rate N, allows the heat flux to be adjusted across a wide range of values, and the kinetic energy to be exchanged in large chunks or more smoothly.
The "middle" layer for velocity swapping is defined as the $Nbin/2 + 1$ layer. Thus if $Nbin = 20$, the two swapping layers are 1 and 11. This should lead to a symmetric temperature profile since the two layers are separated by the same distance in both directions in a periodic sense. This is why $Nbin$ is restricted to being an even number.

As described below, the total kinetic energy transferred by these swaps is computed by the fix and can be output. Dividing this quantity by time and the cross-sectional area of the simulation box yields a heat flux. The ratio of heat flux to the slope of the temperature profile is the thermal conductivity of the fluid, in appropriate units. See the Muller-Plathe paper for details.

IMPORTANT NOTE: After equilibration, if the temperature gradient you observe is not linear, then you are likely swapping energy too frequently and are not in a regime of linear response. In this case you cannot accurately infer a thermal conductivity and should try increasing the Nevery parameter.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cumulative kinetic energy transferred between the bottom and middle of the simulation box (in the edim direction) is stored as a scalar quantity by this fix. This quantity is zeroed when the fix is defined and accumulates thereafter, once every N steps. The units of the quantity are energy; see the units command for details. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

Swaps conserve both momentum and kinetic energy, even if the masses of the swapped atoms are not equal. Thus you should not need to thermostat the system. If you do use a thermostat, you may want to apply it only to the non-swapped dimensions (other than vdim).

LAMMPS does not check, but you should not use this fix to swap the kinetic energy of atoms that are in constrained molecules, e.g. via fix shake or fix rigid. This is because application of the constraints will alter the amount of transferred momentum. You should, however, be able to use flexible molecules. See the Zhang paper for a discussion and results of this idea.

When running a simulation with large, massive particles or molecules in a background solvent, you may want to only exchange kinetic energy between solvent particles.

**Related commands:**

fix ave/spatial, fix viscosity, compute heat/flux

**Default:**

The option defaults are swap = 1.

fix tmd command

Syntax:

fix ID group-ID tmd rho_final file1 N file2

- ID, group-ID are documented in fix command
- tmd = style name of this fix command
- rho_final = desired value of rho at the end of the run (distance units)
- file1 = filename to read target structure from
- N = dump TMD statistics every this many timesteps, 0 = no dump
- file2 = filename to write TMD statistics to (only needed if N > 0)

Examples:

fix 1 all nve
fix 2 tmdatoms tmd 1.0 target_file 100 tmd_dump_file

Description:

Perform targeted molecular dynamics (TMD) on a group of atoms. A holonomic constraint is used to force the atoms to move towards (or away from) the target configuration. The parameter "rho" is monotonically decreased (or increased) from its initial value to rho_final at the end of the run.

Rho has distance units and is a measure of the root-mean-squared distance (RMSD) between the current configuration of the atoms in the group and the target coordinates listed in file1. Thus a value of rho_final = 0.0 means move the atoms all the way to the final structure during the course of the run.

The target file1 can be ASCII text or a gzipped text file (detected by a .gz suffix). The format of the target file1 is as follows:

0.0 25.0 xlo xhi
0.0 25.0 ylo yhi
0.0 25.0 zlo zhi
125 24.97311 1.69005 23.46956 0 0 -1
126 1.94691 2.79640 1.92799 1 0 0
127 0.15906 3.46099 0.79121 1 0 0
...

The first 3 lines may or may not be needed, depending on the format of the atoms to follow. If image flags are included with the atoms, the 1st 3 lo/hi lines must appear in the file. If image flags are not included, the 1st 3 lines should not appear. The 3 lines contain the simulation box dimensions for the atom coordinates, in the same format as in a LAMMPS data file (see the read_data command).

The remaining lines each contain an atom ID and its target x,y,z coordinates. The atom lines (all or none of them) can optionally be followed by 3 integer values: nx,ny,nz. For periodic dimensions, they specify which image of the box the atom is considered to be in, i.e. a value of N (positive or negative) means add N times the box length to the coordinate to get the true value.

The atom lines can be listed in any order, but every atom in the group must be listed in the file. Atoms not in the fix group may also be listed; they will be ignored.
TMD statistics are written to file2 every N timesteps, unless N is specified as 0, which means no statistics.

The atoms in the fix tmd group should be integrated (via a fix nve, nvt, npt) along with other atoms in the system.

Restarts can be used with a fix tmd command. For example, imagine a 10000 timestep run with a rho_initial = 11 and a rho_final = 1. If a restart file was written after 2000 time steps, then the configuration in the file would have a rho value of 9. A new 8000 time step run could be performed with the same rho_final = 1 to complete the conformational change at the same transition rate. Note that for restarted runs, the name of the TMD statistics file should be changed to prevent it being overwritten.

For more information about TMD, see (Schlitter1) and (Schlitter2).

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands.

This fix can ramp its rho parameter over multiple runs, using the start and stop keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

All TMD fixes must be listed in the input script after all integrator fixes (nve, nvt, npt) are applied. This ensures that atoms are moved before their positions are corrected to comply with the constraint.

Atoms that have a TMD fix applied should not be part of a group to which a SHAKE fix is applied. This is because LAMMPS assumes there are not multiple competing holonomic constraints applied to the same atoms.

To read gzipped target files, you must compile LAMMPS with the -DLAMMPS_GZIP option - see the Making LAMMPS section of the documentation.

Related commands: none

Default: none

(Schlitter1) Schlitter, Swegat, Mulders, "Distance-type reaction coordinates for modelling activated processes", J Molecular Modeling, 7, 171-177 (2001).

fix ttm command

Syntax:

fix ID group-ID ttm seed C_e rho_e kappa_e gamma_p gamma_s v_0 Nx Ny Nz T_infile N T_outfile

• ID, group-ID are documented in fix command
• ttm = style name of this fix command
• seed = random number seed to use for white noise (positive integer)
• C_e = electronic specific heat (energy/(electron*temperature) units)
• rho_e = electronic density (electrons/volume units)
• kappa_e = electronic thermal conductivity (energy/(time*distance*temperature) units)
• gamma_p = friction coefficient due to electron-ion interactions (mass/time units)
• gamma_s = friction coefficient due to electronic stopping (mass/time units)
• v_0 = electronic stopping critical velocity (velocity units)
• Nx = number of thermal solve grid points in the x-direction (positive integer)
• Ny = number of thermal solve grid points in the y-direction (positive integer)
• Nz = number of thermal solve grid points in the z-direction (positive integer)
• T_infile = filename to read initial electronic temperature from
• N = dump TTM temperatures every this many timesteps, 0 = no dump
• T_outfile = filename to write TTM temperatures to (only needed if N > 0)

Examples:

fix 2 all ttm 699489 1.0 1.0 10 0.1 0.0 2.0 1 12 1 initialTs 1000 T.out
fix 2 all ttm 123456 1.0 1.0 1.0 1.0 1.0 5.0 5 5 5 Te.in 1 Te.out

Description:

Use a two-temperature model (TTM) to represent heat transfer through and between electronic and atomic subsystems. LAMMPS models the atomic subsystem as usual with a molecular dynamics model and the classical force field specified by the user, but the electronic subsystem is modeled as a continuum, or a background "gas", on a regular grid. Energy can be transferred spatially within the grid representing the electrons. Energy can also be transferred between the electronic and the atomic subsystems. The algorithm underlying this fix was derived by D. M. Duffy and A. M. Rutherford and is discussed in two J Physics: Condensed Matter papers: (Duffy) and (Rutherford). They used this algorithm in cascade simulations where a primary knock-on atom (PKA) was initialized with a high velocity to simulate a radiation event.

Heat transfer between the electronic and atomic subsystems is carried out via an inhomogeneous Langevin thermostat. This thermostat differs from the regular Langevin thermostat (fix langevin) in three important ways. First, the Langevin thermostat is applied uniformly to all atoms in the user-specified group for a single target temperature, whereas the TTM fix applies Langevin thermostatting locally to atoms within the volumes represented by the user-specified grid points with a target temperature specific to that grid point. Second, the Langevin thermostat couples the temperature of the atoms to an infinite heat reservoir, whereas the heat reservoir for fix TTM is finite and represents the local electrons. Third, the TTM fix allows users to specify not just one friction coefficient, but rather two independent friction coefficients: one for the electron-ion interactions (gamma_p), and one for electron stopping (gamma_s).

When the friction coefficient due to electron stopping, gamma_s, is non-zero, electron stopping effects are included for atoms moving faster than the electron stopping critical velocity, v_0. For further details about this
algorithm, see (Duffy) and (Rutherford).

Energy transport within the electronic subsystem is solved according to the heat diffusion equation with added source terms for heat transfer between the subsystems:

\[
C_e \rho_e \frac{\partial T_e}{\partial t} = \nabla (\kappa_e \nabla T_e) - g_p (T_e - T_a) + g_s T_a'
\]

where \(C_e\) is the specific heat, \(\rho_e\) is the density, \(\kappa_e\) is the thermal conductivity, \(T\) is temperature, the "e" and "a" subscripts represent electronic and atomic subsystems respectively, \(g_p\) is the coupling constant for the electron-ion interaction, and \(g_s\) is the electron stopping coupling parameter. \(C_e, \rho_e,\) and \(\kappa_e\) are specified as parameters to the fix. The other quantities are derived. The form of the heat diffusion equation used here is almost the same as that in equation 6 of (Duffy), with the exception that the electronic density is explicitly represented, rather than being part of the the specific heat parameter.

Currently, this fix assumes that none of the user-supplied parameters will vary with temperature. This assumption can be relaxed by modifying the source code to include the desired temperature dependency and functional form for any of the parameters. Note that (Duffy) used a \(\tanh()\) functional form for the temperature dependence of the electronic specific heat, but ignored temperature dependencies of any of the other parameters.

This fix requires use of periodic boundary conditions and a 3D simulation. Periodic boundary conditions are also used in the heat equation solve for the electronic subsystem. This varies from the approach of (Rutherford) where the atomic subsystem was embedded within a larger continuum representation of the electronic subsystem.

The initial electronic temperature input file, \(T_{infile}\), is a text file LAMMPS reads in with no header and with four numeric columns \((ix, iy, iz, Temp)\) and with a number of rows equal to the number of user-specified grid points \((Nx\ by\ Ny\ by\ Nz)\). The \(ix, iy, iz\) are node indices from 0 to \(nxnodes-1\), etc. For example, the initial electronic temperatures on a 1 by 2 by 3 grid could be specified in a \(T_{infile}\) as follows:

\[
\begin{align*}
0 & 0 0 1.0 \\
0 & 0 1 1.0 \\
0 & 0 2 1.0 \\
0 & 1 0 2.0 \\
0 & 1 1 2.0 \\
0 & 1 2 2.0 \\
\end{align*}
\]

where the electronic temperatures along the \(y=0\) plane have been set to 1.0, and the electronic temperatures along the \(y=1\) plane have been set to 2.0. The order of lines in this file is no important. If all the nodal values are not specified, LAMMPS will generate an error.

The temperature output file, \(T_{outfile}\), is created and written by this fix. Temperatures for both the electronic and atomic subsystems at every node and every N timesteps are output. If N is specified as zero, no output is generated, and no output filename is needed. The format of the output is as follows. One long line is written every output timestep. The timestep itself is given in the first column. The next \(N x*N y*N z\) columns contain the temperatures for the atomic subsystem, and the final \(N x*N y*N z\) columns contain the temperatures for the electronic subsystem. The ordering of the \(N x*N y*N z\) columns is with the \(z\) index varying fastest, \(y\) the next fastest, and \(x\) the slowest.

This fix does not change the coordinates of its atoms; it only scales their velocities. Thus a time integration fix (e.g. fix nve) should still be used to time integrate the affected atoms. This fix should not normally be used on
This fix computes 2 output quantities stored in a vector of length 2, which can be accessed by various output commands. The first quantity is the total energy of the electronic subsystem. The second quantity is the energy transferred from the electronic to the atomic subsystem on that timestep. Note that the velocity verlet integrator applies the fix ttm forces to the atomic subsystem as two half-step velocity updates: one on the current timestep and one on the subsequent timestep. Consequently, the change in the atomic subsystem energy is lagged by half a timestep relative to the change in the electronic subsystem energy. As a result of this, users may notice slight fluctuations in the sum of the atomic and electronic subsystem energies reported at the end of the timestep.

The vector values calculated by this fix are "extensive".

IMPORTANT NOTE: The current implementation creates a copy of the electron grid that overlays the entire simulation domain, for each processor. Values on the grid are summed across all processors. Thus you should insure that this grid is not too large, else your simulation could incur high memory and communication costs.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the electronic subsystem and the energy exchange between the subsystems to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Because the state of the random number generator is not saved in the restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix can only be used for 3d simulations and orthogonal simulation boxes. You must use periodic boundary conditions with this fix.

Related commands:

fix langevin, fix dt/reset

Default: none


**fix viscosity command**

**Syntax:**

```
fix ID group-ID viscosity N vdim pdim Nbin keyword value ...
```

- ID, group-ID are documented in fix command
- viscosity = style name of this fix command
- N = perform momentum exchange every N steps
- vdim = x or y or z = which momentum component to exchange
- pdim = x or y or z = direction of momentum transfer
- Nbin = # of layers in pdim direction (must be even number)
- zero or more keyword/value pairs may be appended
- keyword = swap or vtarget

\[\text{swap value} = \text{Nswap} = \text{number of swaps to perform every N steps}\]
\[\text{vtarget value} = V \text{ or INF} = \text{target velocity of swap partners (velocity units)}\]

**Examples:**

```
fix 1 all viscosity 100 x z 20
fix 1 all viscosity 50 x z 20 swap 2 vtarget 1.5
```

**Description:**

Use the Muller-Plathe algorithm described in this paper to exchange momenta between two particles in different regions of the simulation box every N steps. This induces a shear velocity profile in the system. As described below this enables a viscosity of the fluid to be calculated. This algorithm is sometimes called a reverse non-equilibrium MD (reverse NEMD) approach to computing viscosity. This is because the usual NEMD approach is to impose a shear velocity profile on the system and measure the response via an off-diagonal component of the stress tensor, which is proportional to the momentum flux. In the Muller-Plathe method, the momentum flux is imposed, and the shear velocity profile is the system's response.

The simulation box is divided into \(N_{bin}\) layers in the \(pdim\) direction, where the layer 1 is at the low end of that dimension and the layer \(N_{bin}\) is at the high end. Every N steps, Nswap pairs of atoms are chosen in the following manner. Only atoms in the fix group are considered. Nswap atoms in layer 1 with positive velocity components in the \(vdim\) direction closest to the target value \(V\) are selected. Similarly, Nswap atoms in the "middle" layer (see below) with negative velocity components in the \(vdim\) direction closest to the negative of the target value \(V\) are selected. The two sets of Nswap atoms are paired up and their \(vdim\) momenta components are swapped within each pair. This resets their velocities, typically in opposite directions. Over time, this induces a shear velocity profile in the system which can be measured using commands such as the following, which writes the profile to the file tmp.profile:

```
fix f1 all ave/spatial 100 10 1000 z lower 0.05 vx &
    file tmp.profile units reduced
```

Note that by default, Nswap = 1 and vtarget = INF, though this can be changed by the optional swap and vtarget keywords. When vtarget = INF, one or more atoms with the most positive and negative velocity components are selected. Setting these parameters appropriately, in conjunction with the swap rate N, allows the momentum flux rate to be adjusted across a wide range of values, and the momenta to be exchanged in large chunks or more smoothly.
The "middle" layer for momenta swapping is defined as the $N_{bin}/2 + 1$ layer. Thus if $N_{bin} = 20$, the two swapping layers are 1 and 11. This should lead to a symmetric velocity profile since the two layers are separated by the same distance in both directions in a periodic sense. This is why $N_{bin}$ is restricted to being an even number.

As described below, the total momentum transferred by these velocity swaps is computed by the fix and can be output. Dividing this quantity by time and the cross-sectional area of the simulation box yields a momentum flux. The ratio of momentum flux to the slope of the shear velocity profile is the viscosity of the fluid, in appropriate units. See the Muller-Plathe paper for details.

IMPORTANT NOTE: After equilibration, if the velocity profile you observe is not linear, then you are likely swapping momentum too frequently and are not in a regime of linear response. In this case you cannot accurately infer a viscosity and should try increasing the Nevery parameter.

An alternative method for calculating a viscosity is to run a NEMD simulation, as described in Section_howto 13 of the manual. NEMD simulations deform the simulation box via the fix deform command. Thus they cannot be run on a charged system using a PPPM solver since PPPM does not currently support non-orthogonal boxes. Using fix viscosity keeps the box orthogonal; thus it does not suffer from this limitation.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cumulative momentum transferred between the bottom and middle of the simulation box (in the $pdim$ direction) is stored as a scalar quantity by this fix. This quantity is zeroed when the fix is defined and accumulates thereafter, once every N steps. The units of the quantity are momentum = mass*velocity. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

Swaps conserve both momentum and kinetic energy, even if the masses of the swapped atoms are not equal. Thus you should not need to thermostat the system. If you do use a thermostat, you may want to apply it only to the non-swapped dimensions (other than $vdim$).

LAMMPS does not check, but you should not use this fix to swap velocities of atoms that are in constrained molecules, e.g. via fix shake or fix rigid. This is because application of the constraints will alter the amount of transferred momentum. You should, however, be able to use flexible molecules. See the Maginn paper for an example of using this algorithm in a computation of alcohol molecule properties.

When running a simulation with large, massive particles or molecules in a background solvent, you may want to only exchange momenta between solvent particles.

**Related commands:**

fix ave/spatial, fix thermal/conductivity

**Default:**
The option defaults are swap = 1 and vtarget = INF.


fix viscous command

fix viscous/cuda command

Syntax:

fix ID group-ID viscous gamma keyword values ... 

- ID, group-ID are documented in fix command
- viscous = style name of this fix command
- gamma = damping coefficient (force/velocity units)
- zero or more keyword/value pairs may be appended

keyword = scale
    scale values = type ratio
    type = atom type (1-N)
    ratio = factor to scale the damping coefficient by

Examples:

fix 1 flow viscous 0.1
fix 1 damp viscous 0.5 scale 3 2.5

Description:

Add a viscous damping force to atoms in the group that is proportional to the velocity of the atom. The added force can be thought of as a frictional interaction with implicit solvent, i.e. the no-slip Stokes drag on a spherical particle. In granular simulations this can be useful for draining the kinetic energy from the system in a controlled fashion. If used without additional thermostatting (to add kinetic energy to the system), it has the effect of slowly (or rapidly) freezing the system; hence it can also be used as a simple energy minimization technique.

The damping force F is given by F = - gamma * velocity. The larger the coefficient, the faster the kinetic energy is reduced. If the optional keyword scale is used, gamma can scaled up or down by the specified factor for atoms of that type. It can be used multiple times to adjust gamma for several atom types.

IMPORTANT NOTE: You should specify gamma in force/velocity units. This is not the same as mass/time units, at least for some of the LAMMPS units options like "real" or "metal" that are not self-consistent.

In a Brownian dynamics context, gamma = Kb T / D. where Kb = Boltzmann's constant, T = temperature, and D = particle diffusion coefficient. D can be written as Kb T / (3 pi eta d), where eta = dynamic viscosity of the frictional fluid and d = diameter of particle. This means gamma = 3 pi eta d, and thus is proportional to the viscosity of the fluid and the particle diameter.

In the current implementation, rather than have the user specify a viscosity, gamma is specified directly in force/velocity units. If needed, gamma can be adjusted for atoms of different sizes (i.e. sigma) by using the scale keyword.

Note that Brownian dynamics models also typically include a randomized force term to thermostat the system at a chosen temperature. The fix langevin command does this. It has the same viscous damping term as fix viscous and adds a random force to each atom. Hence if using fix langevin you do not typically need to use fix viscous. Also note that the gamma of fix viscous is related to the damping parameter of fix langevin, except that the units
of gamma are force/velocity and the units of damp are time, so that it can more easily be used as a thermostat.

Styles with a \textit{cuda} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in \texttt{Section\_accelerate} of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the \texttt{Making LAMMPS} section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \texttt{-suffix} command-line switch when you invoke LAMMPS, or you can use the \texttt{suffix} command in your input script.

See \texttt{Section\_accelerate} of the manual for more instructions on how to use the accelerated styles effectively.

\textbf{Restart, fix\_modify, output, run start/stop, minimize info:}

No information about this fix is written to binary restart files. None of the \texttt{fix\_modify} options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the \texttt{start/stop} keywords of the \texttt{run} command.

The forces due to this fix are imposed during an energy minimization, invoked by the \texttt{minimize} command. This fix should only be used with damped dynamics minimizers that allow for non-conservative forces. See the \texttt{min\_style} command for details.

\textbf{Restrictions:} none

\textbf{Related commands:}

\texttt{fix langevin}

\textbf{Default:} none
fix wall/lj93 command

fix wall/lj126 command

fix wall/colloid command

fix wall/harmonic command

Syntax:

fix ID group-ID style face args ... keyword value ...

• ID, group-ID are documented in fix command
• style = wall/lj93 or wall/lj126 or wall/colloid or wall/harmonic
• one or more face/arg pairs may be appended
• face = xlo or xhi or ylo or yhi or zlo or zhi

args = coord epsilon sigma cutoff
coord = position of wall = EDGE or constant or variable
EDGE = current lo or hi edge of simulation box
constant = number like 0.0 or -30.0 (distance units)
variable = equal-style variable like v_x or v_wiggle
epsilon = strength factor for wall-particle interaction (energy or energy/distance^2 units)
sigma = size factor for wall-particle interaction (distance units)
cutoff = distance from wall at which wall-particle interaction is cut off (distance units)

• zero or more keyword/value pairs may be appended
• keyword = units or fld

units value = lattice or box
lattice = the wall position is defined in lattice units
box = the wall position is defined in simulation box units
fld value = yes or no
yes = invoke the wall constraint to be compatible with implicit FLD
yes = invoke the wall constraint in the normal way

Examples:

fix wallhi all wall/lj93 xlo -1.0 1.0 1.0 2.5 units box
fix wallhi all wall/lj93 xhi EDGE 1.0 1.0 2.5
fix wallhi all wall/lj126 v_wiggle 23.2 1.0 1.0 2.5
fix zwalls all wall/colloid zlo 0.0 1.0 1.0 0.858 zhi 40.0 1.0 1.0 0.858

Description:

Bound the simulation domain on one or more of its faces with a flat wall that interacts with the atoms in the group by generating a force on the atom in a direction perpendicular to the wall. The energy of wall-particle interactions depends on the style.

For style wall/lj93, the energy E is given by the 9/3 potential:
For style `wall/lj126`, the energy $E$ is given by the 12/6 potential:

$$E = \epsilon \left[ \frac{2}{15} \left( \frac{\sigma}{r} \right)^9 - \left( \frac{\sigma}{r} \right)^3 \right] \quad r < r_c$$

For style `wall/collloid`, the energy $E$ is given by an integrated form of the `pair_style colloid` potential:

$$E = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad r < r_c$$

For style `wall/harmonic`, the energy $E$ is given by a harmonic spring potential:

$$E = 144\phi^2 \epsilon \left[ \frac{\sigma^6}{7560} \left( \frac{6R - D}{D^7} + \frac{D + 8R}{(D + 2R)^7} \right) - \frac{1}{6} \left( \frac{2R(D + R) + D(D + 2R) [\ln D - \ln(D + 2R)]}{D(D + 2R)} \right) \right] \quad r <$$

In all cases, $r$ is the distance from the particle to the wall at position `coord`, and $r_c$ is the cutoff distance at which the particle and wall no longer interact. The energy of the wall potential is shifted so that the wall-particle interaction energy is 0.0 at the cutoff distance.

Up to 6 walls or faces can be specified in a single command: `xlo`, `xhi`, `ylo`, `yhi`, `zlo`, `zhi`. A `lo` face interacts with particles near the lower side of the simulation box in that dimension. A `hi` face interacts with particles near the upper side of the simulation box in that dimension.

The position of each wall can be specified in one of 3 ways: as the EDGE of the simulation box, as a constant value, or as a variable. If `EDGE` is used, then the corresponding boundary of the current simulation box is used. If a numeric constant is specified then the wall is placed at that position in the appropriate dimension (x, y, or z). In both the `EDGE` and constant cases, the wall will never move. If the wall position is a variable, it should be specified as `v_name`, where name is an equal-style variable name. In this case the variable is evaluated each timestep and the result becomes the current position of the reflecting wall. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position. See examples below.
For the `wall/lj93` and `wall/lj126` styles, `epsilon` and `sigma` are the usual Lennard-Jones parameters, which determine the strength and size of the particle as it interacts with the wall. Epsilon has energy units. Note that this `epsilon` and `sigma` may be different than any `epsilon` or `sigma` values defined for a pair style that computes particle-particle interactions.

The `wall/lj93` interaction is derived by integrating over a 3d half-lattice of Lennard-Jones 12/6 particles. The `wall/lj126` interaction is effectively a harder, more repulsive wall interaction.

For the `wall/collloid` style, `epsilon` is effectively a Hamaker constant with energy units for the colloid-wall interaction, \( R \) is the radius of the colloid particle, \( D \) is the distance from the surface of the colloid particle to the wall (\( r-R \)), and `sigma` is the size of a constituent LJ particle inside the colloid particle. Note that the cutoff distance \( R_c \) in this case is the distance from the colloid particle center to the wall.

The `wall/collloid` interaction is derived by integrating over constituent LJ particles of size `sigma` within the colloid particle and a 3d half-lattice of Lennard-Jones 12/6 particles of size `sigma` in the wall.

For the `wall/harmonic` style, `epsilon` is effectively the spring constant \( K \), and has units \((\text{energy/distance}^2)\). The input parameter `sigma` is ignored. The minimum energy position of the harmonic spring is at the `cutoff`. This is a repulsive-only spring since the interaction is truncated at the `cutoff`.

IMPORTANT NOTE: For all of the styles, you must insure that \( r \) is always \( > 0 \) for all particles in the group, or LAMMPS will generate an error. This means you cannot start your simulation with particles at the wall position `coord` (\( r = 0 \)) or with particles on the wrong side of the wall (\( r < 0 \)). For the `wall/lj93` and `wall/lj126` styles, the energy of the wall/particle interaction (and hence the force on the particle) blows up as \( r \rightarrow 0 \). The `wall/collloid` style is even more restrictive, since the energy blows up as \( D = r-R \rightarrow 0 \). This means the finite-size particles of radius \( R \) must be a distance larger than \( R \) from the wall position `coord`. The `harmonic` style is a softer potential and does not blow up as \( r \rightarrow 0 \), but you must use a large enough `epsilon` that particles always remain on the correct side of the wall (\( r > 0 \)).

The `units` keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant or variable is used. It is not relevant when `EDGE` is used to specify a face position. In the variable case, the variable is assumed to produce a value compatible with the `units` setting you specify.

A `box` value selects standard distance units as defined by the `units` command, e.g. Angstroms for `units = real` or metal. A `lattice` value means the distance units are in lattice spacings. The `lattice` command must have been previously used to define the lattice spacings.

The `fld` keyword can be used with a `yes` setting to invoke the wall constraint before pairwise interactions are computed. This allows an implicit FLD model using `pair_style lubricateU` to include the wall force in its calculations. If the setting is `no`, wall forces are imposed after pairwise interactions, in the usual manner.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using equal-style `variables`.

```
variable ramp equal ramp(0,10)
fix 1 all wall xlo v_ramp 1.0 1.0 2.5

variable linear equal vdisplace(0,20)
fix 1 all wall xlo v_linear 1.0 1.0 2.5

variable wiggle equal swiggle(0.0,5.0,3.0)
fix 1 all wall xlo v_wiggle 1.0 1.0 2.5

variable wiggle equal cwiggle(0.0,5.0,3.0)
```
fix 1 all wall xlo v_wiggle 1.0 1.0 2.5

The ramp(lo,hi) function adjusts the wall position linearly from lo to hi over the course of a run. The vdisplace(c0,velocity) function does something similar using the equation position = c0 + velocity*delta, where delta is the elapsed time.

The swiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, where omega = 2 PI / period:

\[ \text{position} = c0 + A \sin(\omega \delta) \]

The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

\[ \text{position} = c0 + A \left( 1 - \cos(\omega \delta) \right) \]

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files.

The `fix_modify energy` option is supported by this fix to add the energy of interaction between atoms and each wall to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar energy and a global vector of forces, which can be accessed by various output commands. Note that the scalar energy is the sum of interactions with all defined walls. If you want the energy on a per-wall basis, you need to use multiple fix wall commands. The length of the vector is equal to the number of walls defined by the fix. Each vector value is the normal force on a specific wall. Note that an outward force on a wall will be a negative value for `lo` walls and a positive value for `hi` walls. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the `start/stop` keywords of the `run` command.

The forces due to this fix are imposed during an energy minimization, invoked by the `minimize` command.

IMPORTANT NOTE: If you want the atom/wall interaction energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the `fix_modify energy` option for this fix.

**Restrictions:**

Any dimension (xyz) that has a wall must be non-periodic.

**Related commands:**

`fix wall/reflect`, `fix wall/gran`, `fix wall/region`

**Default:**

The option defaults are no velocity, no wiggle, and units = lattice.
**fix wall/gran command**

**Syntax:**

```
fix ID group-ID wall/gran Kn Kt gamma_n gamma_t xmu dampflag style args ... keyword values ...
```

- ID, group-ID are documented in fix command
- wall/gran = style name of this fix command
- Kn = elastic constant for normal particle repulsion (force/distance units or pressure units - see discussion below)
- Kt = elastic constant for tangential contact (force/distance units or pressure units - see discussion below)
- gamma_n = damping coefficient for collisions in normal direction (1/time units or 1/time-distance units - see discussion below)
- gamma_t = damping coefficient for collisions in tangential direction (1/time units or 1/time-distance units - see discussion below)
- xmu = static yield criterion (unitless fraction between 0.0 and 1.0)
- dampflag = 0 or 1 if tangential damping force is excluded or included
- one or more style/arg pairs may be appended
- style = xlo or xhi or ylo or yhi or zlo or zhi or zcylinder
- args = list of arguments for a particular style

```
xlo or xhi or ylo or yhi or zlo or zhi args = coord vwall
coord = position of wall = constant or variable
  constant = number like 0.0 or -30.0 (distance units)
  variable = equal-style variable like v_x or v_wiggle
vwall = velocity of wall in normal direction = constant or variable
  constant = number like 0.0 or 2.0 (velocity units)
  variable = equal-style variable like v_vx or v_wiggle
zcylinder args = rad vrad
  rad = radius of cylinder = constant or variable
  constant = number like 0.0 or -30.0 (distance units)
  variable = equal-style variable like v_rad or v_wiggle
vwall = velocity of radius in normal direction = constant or variable
  constant = number like 0.0 or 2.0 (velocity units)
  variable = equal-style variable like v_vrad or v_wiggle
```

- zero or more keyword/value pairs may be appended to args
- keyword = shear or piston

```
shear values = dim vshear
  dim = x or y or z or theta
  vshear = shear velocity = constant or variable
    constant = number like 2.0 or -2.0 (velocity units or radians/time units)
    variable = equal-style variable like v_vshear or v_wiggle
piston values = pload pmass
  pload = external load on piston = constant or variable
    constant = number like 0.0 or 30.0 (force units)
    variable = equal-style variable like v_push or v_wiggle
  pmass = piston mass (mass units)
```

**Examples:**

```
fix 1 all wall/gran 200000.0 NULL 50.0 NULL 0.5 0 xlo -10.0 0 xhi 10.0 0
fix 1 all wall/gran 200000.0 NULL 50.0 NULL 0.5 0 zhi v_squeeze shear x v_ramp
fix 2 all wall/gran 100000.0 20000.0 50.0 30.0 0.5 1 zcylinder 15.0 0.0 piston -5000.0 1000.0
```
Description:

Bound the simulation domain of a granular system with one or more frictional walls. All particles in the group interact with the wall when they are close enough to touch it.

The first set of parameters \((K_n, K_t, \gamma_n, \gamma_t, xmu, \text{and} \, \text{dampflag})\) have the same meaning as those specified with the pair_style granular force fields. This means a NULL can be used for either \(K_t\) or \(\gamma_t\) as described on that page. If a NULL is used for \(K_t\), then a default value is used where \(K_t = \frac{2}{7} \, K_n\). If a NULL is used for \(\gamma_t\), then a default value is used where \(\gamma_t = \frac{1}{2} \, \gamma_n\).

The nature of the wall/particle interactions are determined by which pair_style is used in your input script: hooke, hooke/history, or hertz/history. The equation for the force between the wall and particles touching it is the same as the corresponding equation on the pair_style granular doc page, in the limit of one of the two particles going to infinite radius and mass (flat wall). I.e. \(\delta = \text{radius} - r = \text{overlap of particle with wall, } m_{\text{eff}} = \text{mass of particle, } \sqrt{R_iR_j/R_i+R_j}\) becomes \(\sqrt{\text{radius of particle}}\). The units for \(K_n\), \(K_t\), \(\gamma_n\), and \(\gamma_t\) are as described on that doc page. The meaning of \(xmu\) and \(\text{dampflag}\) are also as described on that page. Note that you can choose different values for these 6 wall/particle coefficients than for particle/particle interactions, if you wish your wall to interact differently with the particles, e.g. if the wall is a different material.

IMPORTANT NOTE: As discussed on the doc page for pair_style granular, versions of LAMMPS before 9Jan09 used a different equation for Hertzian interactions. This means Hertzian wall/particle interactions have also changed. They now include a \(\sqrt{\text{radius}}\) term which was not present before. Also the previous versions used \(K_n\) and \(K_t\) from the pairwise interaction and hardwired \(\text{dampflag}\) to 1, rather than letting them be specified directly. This means you can set the values of the wall/particle coefficients appropriately in the current code to reproduce the results of a previous Hertzian monodisperse calculation. For example, for the common case of a monodisperse system with particles of diameter 1, \(K_n\), \(K_t\), \(\gamma_n\), and \(\gamma_s\) should be set \(\sqrt{2.0}\) larger than they were previously.

One or more wall styles can be specified. The \(xlo, xhi, ylo, yhi, zlo, zhi\) styles are planar faces that push particles back into the box from one of their sides. E.g. the \(xlo\) wall should be positioned to the left of all particles in the x dimension, so that it pushes particles to the right, and conversely for the \(xhi\) wall. The \(zcylinder\) style is a cylindrical shell with its axis along the z-axis, centered at \(x = y = 0.0\). The interior surface of the cylinder pushes particles towards the \(x = y = 0.0\) center axis. The \(zcylinder\) style cannot be specified with any of the \(xlo, xhi, ylo, yhi\) styles, but if can be with the \(zlo\) or \(zhi\) styles.

For the planer wall styles, \(coord\) and \(vwall\) arguments are specified. These are the position and normal velocity of the wall. A positive velocity means the wall is moving in the positive direction in the normal dimension, e.g. +x for a \(xlo\) or \(xhi\) wall. Either or both of the \(coord\) and \(vwall\) arguments can be specified as a constant value or a variable. Note that the force exerted by a wall on granular particles depends on the velocity of the wall, in both the normal and tangential directions, so it is important to set \(vwall\) consistent with the \(coord\) argument.

If a numeric constant is specified for \(coord\) then the wall is placed at that position in the appropriate dimension (x, y, or z) and will never move. Likewise if a constant is specified for \(vwall\), then the normal velocity of the wall is set to that value and will never change.

If \(coord\) or \(vwall\) is a variable, it should be specified as \(v\_name\), where name is an equal-style variable name. In this case the variable is evaluated each timestep and the result becomes the current position or normal velocity of the wall. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position and velocity.
If \textit{coord} is specified as a constant, then \textit{vwall} must be specified as 0.0. If \textit{coord} is specified as a variable, then \textit{vwall} must be a non-zero constant or a variable. If \textit{vwall} is specified as a non-zero constant or variable and \textit{coord} as a constant, then \textit{coord} is treated as the initial position of the wall, and the wall position is updated each timestep by \(\text{dt}*\text{v\_current}\), where \(\text{dt}\) = the timestep, and \(\text{v\_current}\) = the current normal velocity.

For the \textit{zcylinder} wall style, \textit{rad} and \textit{vrad} arguments are specified. These are the radius and radial velocity of the cylinder. A positive velocity means the radius is growing. Either or both of the \textit{rad} and \textit{vrad} arguments can be specified as a constant value or a variable. Note that the force exerted by the wall of the cylinder on granular particles depends on the velocity of the wall, in both the normal (radial) and tangential directions, so it is important to set \textit{vrad} consistent with the \textit{rad} argument.

If a numeric constant is specified for \textit{rad} then the cylinder will have a fixed radius. Likewise if a constant is specified for \textit{vrad}, then the radial velocity of the cylinder is set to that value and will never change.

If \textit{rad} or \textit{vrad} is a variable, it should be specified as \textit{v\_name}, where \textit{name} is an equal-style variable name. In this case the variable is evaluated each timestep and the result becomes the current radius or radial velocity of the cylinder. Equal-style variables can specify formulas with various mathematical functions, and include \texttt{thermo\_style} command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent cylinder radius and velocity.

If \textit{rad} is specified as a constant, then \textit{vrad} must be specified as 0.0. If \textit{rad} is specified as a variable, then \textit{vrad} must be a non-zero constant or a variable. If \textit{vrad} is specified as a non-zero constant or variable and \textit{rad} as a constant, then \textit{rad} is treated as the initial radius of the wall, and the radius is updated each timestep by \(\text{dt}*\text{v\_current}\), where \(\text{dt}\) = the timestep, and \(\text{v\_current}\) = the current radial velocity.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using equal-style variables. They also specify the correct normal velocity of the wall based on the time derivative of the position.

\begin{verbatim}
variable ramp equal ramp(0,10)
variable vnorm equal 10/(10000*dt)  # 10000 step run
fix 1 all wall/gran ... xlo v_ramp v_vnorm

variable linear equal vdisplace(0,20)
fix 1 all wall/gran ... xlo v_linear 20

variable omega equal 2*PI/3.0
variable wiggle equal swiggle(0.0,5.0,3.0)
variable vwiggle equal "5.0 * v_omega * cos(v_omega*(timestep-startstep)*dt)"
fix 1 all wall/gran ... xlo v_wiggle v_vwiggle

variable omega equal 2*PI/3.0
variable wiggle equal cwiggle(0.0,5.0,3.0)
variable vwiggle equal "5.0 * v_omega * sin(v_omega*(timestep-startstep)*dt)"
fix 1 all wall/gran ... xlo v_wiggle v_vwiggle
\end{verbatim}

The \texttt{ramp(lo,hi)} function adjusts the wall position linearly from \textit{lo} to \textit{hi} over the course of a run. The \texttt{vdisplace(c0,velocity)} function does something similar using the equation \(\text{position} = \text{c0} + \text{velocity}\*\text{delta}\), where \textit{delta} is the elapsed time.

The \texttt{swiggle(c0,A,period)} function causes the wall position to oscillate sinusoidally according to this equation, where \textit{omega} = 2 PI / \textit{period}:

\begin{verbatim}
position = \text{c0} + A \sin(\text{omega}\*\text{delta})
\end{verbatim}
The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

\[
\text{position} = c0 + A \left(1 - \cos(\omega \delta)\right)
\]

The optional keywords \textit{shear} and \textit{piston} are applied to all the specified wall styles. If you need to apply different options to different wall styles, then you should use multiple fix wall/gran commands.

The \textit{shear} keyword allows specification of one or two tangential velocities for planar or \textit{zcylinder} walls. The \textit{dim} value specifies the velocity direction. \textit{X}, \textit{y}, and \textit{z} can be used for planar walls, but not for the direction normal to the wall. \textit{Z} and \textit{theta} can be used for a \textit{zcylinder} wall. \textit{Theta} is the azimuthal angle in the \textit{xy} plane, i.e. a rotation of the cylinder about its vertical \textit{z} axis. Note that a positive \textit{theta} velocity means increasing \textit{theta}, i.e. rotation in a counter-clockwise direction when looking down on the \textit{xy} plane from above.

\textit{Vshear} is the magnitude of the shear velocity and can be specified as a numeric constant or variable. The units of \textit{vshear} are velocity units for \textit{dim} = \textit{x}, \textit{y}, or \textit{z}. They are units of radians/time for \textit{dim} = \textit{theta}.

If a numeric constant is used, then then the shear velocity will never change. If \textit{vshear} is a variable, it should be specified as \textit{v\_name}, where \textit{name} is an \textit{equal-style variable} name. In this case the variable is evaluated each timestep and the result becomes the current shear velocity. Equal-style variables can specify formulas with various mathematical functions, and include \textit{thermo_style} command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent shear velocity.

The \textit{piston} keyword allows specification of an external loading force on the wall, which is opposed by granular particles pushing back against the load. The wall position and normal velocity adjust dynamically in response to these 2 opposing forces.

\textit{Pload} is the magnitude of the loading force and can be specified as a numeric constant or variable. This force must have a value less than 0.0 which means that it is directed inward towards the particles. Thus for a \textit{xlo} wall, a negative values is a force in the +\textit{x} direction. For a \textit{xhi} wall a negative values is a force in the -\textit{x} direction. For a \textit{zcylinder} wall, a negative value is a force towards the center \textit{z} axis of the cylinder.

If a numeric constant is used for \textit{pload}, then then the load force will never change. If \textit{pload} is a variable, it should be specified as \textit{v\_name}, where \textit{name} is an \textit{equal-style variable} name. In this case the variable is evaluated each timestep and the result becomes the current load force. Equal-style variables can specify formulas with various mathematical functions, and include \textit{thermo_style} command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent load force.

When the \textit{piston} keyword is used, the \textit{coord} and \textit{vwall} argumnets for each wall style (or \textit{rad} and \textit{vrad} arguments for a \textit{zcylinder} style) must be numeric constants and are treated as initial values of the position/radius and velocity/radial-velocity. The initial values are updated every timestep by integrating these equations in a velocity-Verlet fashion:

\[
\begin{align*}
\text{vwall\_new} &= \text{vwall} + \text{dt} \times \left(\text{Fload} + \text{Fparticles}\right) / \text{pmass} \\
\text{xwall\_new} &= \text{xwall} + \text{dt} \times \text{vwall\_new}
\end{align*}
\]

\textit{Fload} and \textit{Fparticles} are the force on the wall due to the external load and interactions with particles respectively. \textit{Fparticles} is always a positive value, representing particles pushing outward on the wall (-\textit{x} direction for a \textit{xlo} wall, +\textit{x} direction for a \textit{xhi} wall, radially outward for a \textit{zcylinder} wall). Thus \textit{Fload} and \textit{Fparticles} will always have opposite signs. \textit{Pmass} is the mass of the wall, as specified with the \textit{piston} keyword. \textit{Xwall} and \textit{Vwall} are the wall position (or radius) and normal velocity (or radial velocity) on the previous timestep. \textit{Xwall\_new} and \textit{vwall\_new} are the updated values.
Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the shear friction state of atoms interacting with the wall to binary restart files, so that a simulation can continue correctly if granular potentials with shear "history" effects are being used. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix does not write any information about the walls (e.g., position or velocity) to the restart file. It is up to you to insure that fix wall/gran commands you re-specify in a restart input script are consistent with the previous simulation.

None of the fix_modify options are relevant to this fix.

This fix computes a global vector of values, which can be accessed by various output commands. The length of the vector is 4*Nstyle, where Nstyle is the number of styles specified.

The 4 values (per style) are as follows:

1. position (or radius) of wall (distance units)
2. normal (or radial) velocity of wall (velocity or radians/time units)
3. positive force on wall due to particles (force units)
4. negative force on wall due to external load (force units)

The sign conventions for these values are as described above. The 4th value will be 0.0 if the piston keyword is not used. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Any dimension (xyz) that has a granular wall must be non-periodic.

Related commands:

fix_move, pair_style granular

Default:

The default shear velocities are 0.0.
fix wall/piston command

Syntax:

fix ID group-ID wall/piston face ... keyword value ...

- ID, group-ID are documented in fix command
- wall/piston = style name of this fix command
- face = zlo
- zero or more keyword/value pairs may be appended
- keyword = pos or vel or ramp or units

pos args = z
  z = z coordinate at which the piston begins (distance units)
vel args = vz
  vz = final velocity of the piston (velocity units)
ramp = use a linear velocity ramp from 0 to vz
temp args = target damp seed extent
  target = target velocity for region immediately ahead of the piston
  damp = damping parameter (time units)
  seed = random number seed for langevin kicks
  extent = extent of thermostated region (distance units)
units value = lattice or box
  lattice = the wall position is defined in lattice units
  box = the wall position is defined in simulation box units

Examples:

fix xwalls all wall/piston zlo
fix walls all wall/piston zlo pos 1.0 0.0 0.0 vel 0.0 0.0 10.0 units box
fix top all wall/piston zlo vel 0.0 0.0 10.0 ramp

Description:

Bound the simulation with a moving wall which reflect particles in the specified group and drive the system with an effective infinite-mass piston capable of driving shock waves.

A momentum mirror technique is used, which means that if an atom (or the wall) moves such that an atom is outside the wall on a timestep by a distance delta (e.g. due to fix nve), then it is put back inside the face by the same delta, and the velocity relative to the moving wall is flipped in z. For instance, a stationary particle hit with a piston wall with velocity vz, will end the timestep with a velocity of 2*vz.

Currently the face keyword can only be zlo. This creates a piston moving in the positive z direction. Particles with z coordinate less than the wall position are reflected to a z coordinate greater than the wall position. If the piston velocity is vpz and the particle velocity before reflection is vzi, the particle velocity after reflection is -vzi + 2*vpz.

The initial position of the wall can be specified by the pos keyword.

The final velocity of the wall can be specified by the vel keyword.

The ramp keyword will cause the wall/piston to adjust the velocity linearly from zero velocity to vel over the course of the run. If the ramp keyword is omitted then the wall/piston moves at a constant velocity defined by vel.
The temp keyword will cause the region immediately in front of the wall/piston to be thermostated with a Langevin thermostat. This region moves with the piston. The damping and kicking are measured in the reference frame of the piston. So, a temperature of zero would mean all particles were moving at exactly the speed of the wall/piston.

The units keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant is used.

A box value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A lattice value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacings.

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The face that has the wall/piston must be boundary type 's' (shrink-wrapped). The opposing face can be any boundary type other than periodic.

A wall/piston should not be used with rigid bodies such as those defined by a "fix rigid" command. This is because the wall/piston displaces atoms directly rather than exerting a force on them.

**Related commands:**

fix wall/reflect command, fix append/atoms command

**Default:**

The keyword defaults are pos = 0, vel = 0, units = lattice.
fix wall/reflect command

Syntax:

fix ID group-ID wall/reflect face arg ... keyword value ...

• ID, group-ID are documented in fix command
• wall/reflect = style name of this fix command
• one or more face/arg pairs may be appended
• face = xlo or xhi or ylo or yhi or zlo or zhi

xlo,ylo,zlo arg = EDGE or constant or variable
  EDGE = current lo edge of simulation box
  constant = number like 0.0 or -30.0 (distance units)
  variable = equal-style variable like v_x or v_wiggle

xhi,yhi,zhi arg = EDGE or constant or variable
  EDGE = current hi edge of simulation box
  constant = number like 50.0 or 100.3 (distance units)
  variable = equal-style variable like v_x or v_wiggle

• zero or more keyword/value pairs may be appended
• keyword = units
  units value = lattice or box
  lattice = the wall position is defined in lattice units
  box = the wall position is defined in simulation box units

Examples:

fix xwalls all wall/reflect xlo EDGE xhi EDGE
fix walls all wall/reflect xlo 0.0 ylo 10.0 units box
fix top all wall/reflect zhi v_pressdown

Description:

Bound the simulation with one or more walls which reflect particles in the specified group when they attempt to
move thru them.

Reflection means that if an atom moves outside the wall on a timestep by a distance delta (e.g. due to fix nve),
then it is put back inside the face by the same delta, and the sign of the corresponding component of its velocity is
flipped.

When used in conjunction with fix nve and run_style verlet, the resultant time-integration algorithm is equivalent
to the primitive splitting algorithm (PSA) described by Bond. Because each reflection event divides the
corresponding timestep asymmetrically, energy conservation is only satisfied to O(dt), rather than to O(dt^2) as it
would be for velocity-Verlet integration without reflective walls.

Up to 6 walls or faces can be specified in a single command: xlo, xhi, ylo, yhi, zlo, zhi. A lo face reflects particles
that move to a coordinate less than the wall position, back in the hi direction. A hi face reflects particles that move
to a coordinate higher than the wall position, back in the lo direction.

The position of each wall can be specified in one of 3 ways: as the EDGE of the simulation box, as a constant
value, or as a variable. If EDGE is used, then the corresponding boundary of the current simulation box is used. If
a numeric constant is specified then the wall is placed at that position in the appropriate dimension (x, y, or z). In
both the EDGE and constant cases, the wall will never move. If the wall position is a variable, it should be
specified as v_name, where name is an equal-style variable name. In this case the variable is evaluated each
timestep and the result becomes the current position of the reflecting wall. Equal-style variables can specify
formulas with various mathematical functions, and include thermo_style command keywords for the simulation
box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position.

The units keyword determines the meaning of the distance units used to define a wall position, but only when a
numeric constant or variable is used. It is not relevant when EDGE is used to specify a face position. In the
variable case, the variable is assumed to produce a value compatible with the units setting you specify.

A box value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or
metal. A lattice value means the distance units are in lattice spacings. The lattice command must have been
previously used to define the lattice spacings.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using
equal-style variables.

```plaintext
variable ramp equal ramp(0,10)
fix 1 all wall/reflect xlo v_ramp

variable linear equal vdisplace(0,20)
fix 1 all wall/reflect xlo v_linear

variable wiggle equal swiggle(0.0,5.0,3.0)
fix 1 all wall/reflect xlo v_wiggle

variable wiggle equal cwiggle(0.0,5.0,3.0)
fix 1 all wall/reflect xlo v_wiggle
```

The ramp(lo,hi) function adjusts the wall position linearly from lo to hi over the course of a run. The
vdisplace(c0,velocity) function does something similar using the equation position = c0 + velocity*delta, where
delta is the elapsed time.

The swiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation,
where omega = 2 PI / period:

```plaintext
position = c0 + A sin(omega*delta)
```

The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation,
which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

```plaintext
position = c0 + A (1 - cos(omega*delta))
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this
fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter
of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy
minimization.

Restrictions:

Any dimension (xyz) that has a reflecting wall must be non-periodic.
A reflecting wall should not be used with rigid bodies such as those defined by a "fix rigid" command. This is because the wall/reflect displaces atoms directly rather than exerts a force on them. For rigid bodies, use a soft wall instead, such as fix wall/lj93. LAMMPS will flag the use of a rigid fix with fix wall/reflect with a warning, but will not generate an error.

**Related commands:**

fix wall/lj93 command

**Default:** none

fix wall/region command

Syntax:

fix ID group-ID wall/region region-ID style epsilon sigma cutoff

• ID, group-ID are documented in fix command
• wall/region = style name of this fix command
• region-ID = region whose boundary will act as wall
• style = lj93 or lj126 or colloid or harmonic
• epsilon = strength factor for wall-particle interaction (energy or energy/distance^2 units)
• sigma = size factor for wall-particle interaction (distance units)
• cutoff = distance from wall at which wall-particle interaction is cut off (distance units)

Examples:

fix wall all wall/region mySphere lj93 1.0 1.0 2.5

Description:

Treat the surface of the geometric region defined by the region-ID as a bounding wall which interacts with nearby particles according to the specified style. The distance between a particle and the surface is the distance to the nearest point on the surface and the force the wall exerts on the particle is along the direction between that point and the particle, which is the direction normal to the surface at that point.

Regions are defined using the region command. Note that the region volume can be interior or exterior to the bounding surface, which will determine in which direction the surface interacts with particles, i.e. the direction of the surface normal. Regions can either be primitive shapes (block, sphere, cylinder, etc) or combinations of primitive shapes specified via the union or intersect region styles. These latter styles can be used to construct particle containers with complex shapes. Regions can also change over time via keywords like linear, wiggle, and rotate, which when used with this fix, have the effect of moving the region surface in a prescribed manner.

IMPORTANT NOTE: As discussed on the region command doc page, regions in LAMMPS do not get wrapped across periodic boundaries. It is up to you to insure that periodic or non-periodic boundaries are specified appropriately via the boundary command when using a region as a wall that bounds particle motion. This also means that if you embed a region in your simulation box and want it to repulse particles from its surface (using the "side out" option in the region command), that its repulsive force will not be felt across a periodic boundary.

IMPORTANT NOTE: For primitive regions with sharp corners and/or edges (e.g. a block or cylinder), wall/particle forces are computed accurately for both interior and exterior regions. For union and intersect regions, additional sharp corners and edges may be present due to the intersection of the surfaces of 2 or more primitive volumes. These corners and edges can be of two types: concave or convex. Concave points/edges are like the corners of a cube as seen by particles in the interior of a cube. Wall/particle forces around these features are computed correctly. Convex points/edges are like the corners of a cube as seen by particles exterior to the cube, i.e. the points jut into the volume where particles are present. LAMMPS does NOT compute the location of these convex points directly, and hence wall/particle forces in the cutoff volume around these points suffer from inaccuracies. The basic problem is that the outward normal of the surface is not continuous at these points. This can cause particles to feel no force (they don't "see" the wall) when in one location, then move a distance epsilon, and suddenly feel a large force because they now "see" the wall. In the worst-case scenario, this can blow particles out of the simulation box. Thus, as a general rule you should not use the fix wall/region command with
union or intersect regions that have convex points or edges.

The energy of wall-particle interactions depends on the specified style.

For style \textit{lj93}, the energy \( E \) is given by the 9/3 potential:

\[
E = \epsilon \left[ \frac{2}{15} \left( \frac{\sigma}{r} \right)^9 - \left( \frac{\sigma}{r} \right)^3 \right] \quad r < r_c
\]

For style \textit{lj126}, the energy \( E \) is given by the 12/6 potential:

\[
E = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad r < r_c
\]

For style \textit{colloid}, the energy \( E \) is given by an integrated form of the \texttt{pair_style colloid} potential:

\[
E = 144 \phi^2 \epsilon \left[ \frac{\sigma^6}{7560} \left( \frac{6R - D}{D^7} + \frac{D + 8R}{(D + 2R)^7} \right) - \frac{1}{6} \left( \frac{2R(D + R) + D(D + 2R) [\ln D - \ln(D + 2R)]}{D(D + 2R)} \right) \right] \quad r < r_c
\]

For style \textit{wall/harmonic}, the energy \( E \) is given by a harmonic spring potential:

\[
E = \epsilon (r - r_c)^2 \quad r < r_c
\]

In all cases, \( r \) is the distance from the particle to the region surface, and \( R_c \) is the cutoff distance at which the particle and surface no longer interact. The energy of the wall potential is shifted so that the wall-particle interaction energy is 0.0 at the cutoff distance.

For the \textit{lj93} and \textit{lj126} styles, \textit{epsilon} and \textit{sigma} are the usual Lennard-Jones parameters, which determine the strength and size of the particle as it interacts with the wall. Epsilon has energy units. Note that this \textit{epsilon} and \textit{sigma} may be different than any \textit{epsilon} or \textit{sigma} values defined for a pair style that computes particle-particle interactions.

The \textit{lj93} interaction is derived by integrating over a 3d half-lattice of Lennard-Jones 12/6 particles. The \textit{lj126} interaction is effectively a harder, more repulsive wall interaction.
For the *colloid* style, *epsilon* is effectively a Hamaker constant with energy units for the colloid-wall interaction, \( R \) is the radius of the colloid particle, \( D \) is the distance from the surface of the colloid particle to the wall \( (r-R) \), and *sigma* is the size of a constituent LJ particle inside the colloid particle. Note that the cutoff distance \( R_c \) in this case is the distance from the colloid particle center to the wall.

The *colloid* interaction is derived by integrating over constituent LJ particles of size *sigma* within the colloid particle and a 3d half-lattice of Lennard-Jones 12/6 particles of size *sigma* in the wall.

For the *wall/harmonic* style, *epsilon* is effectively the spring constant \( K \), and has units \( \text{energy/distance}^2 \). The input parameter *sigma* is ignored. The minimum energy position of the harmonic spring is at the *cutoff*. This is a repulsive-only spring since the interaction is truncated at the *cutoff*.

IMPORTANT NOTE: For all of the styles, you must insure that \( r \) is always \( > 0 \) for all particles in the group, or LAMMPS will generate an error. This means you cannot start your simulation with particles on the region surface \( (r = 0) \) or with particles on the wrong side of the region surface \( (r < 0) \). For the *wall/lj93* and *wall/lj126* styles, the energy of the wall/particle interaction (and hence the force on the particle) blows up as \( r \rightarrow 0 \). The *wall/colloid* style is even more restrictive, since the energy blows up as \( D = r-R \rightarrow 0 \). This means the finite-size particles of radius \( R \) must be a distance larger than \( R \) from the region surface. The *harmonic* style is a softer potential and does not blow up as \( r \rightarrow 0 \), but you must use a large enough *epsilon* that particles always remain on the correct side of the region surface \( (r > 0) \).

**Restrictions:** none

**Related commands:**

*fix wall/lj93, fix wall/lj126, fix wall/colloid, fix wall/gran*

**Default:** none
fix wall/srd command

Syntax:

fix ID group-ID wall/srd face arg ... keyword value ...

- ID, group-ID are documented in fix command
- wall/srd = style name of this fix command
- one or more face/arg pairs may be appended
- face = xlo or xhi or ylo or yhi or zlo or zhi

xlo,ylo,zlo arg = EDGE or constant or variable
  EDGE = current lo edge of simulation box
  constant = number like 0.0 or -30.0 (distance units)
  variable = equal-style variable like v_x or v_wiggle

xhi,yhi,zhi arg = EDGE or constant or variable
  EDGE = current hi edge of simulation box
  constant = number like 50.0 or 100.3 (distance units)
  variable = equal-style variable like v_x or v_wiggle

- zero or more keyword/value pairs may be appended
- keyword = units
  units value = lattice or box
    lattice = the wall position is defined in lattice units
    box = the wall position is defined in simulation box units

Examples:

fix xwalls all wall/srd xlo EDGE xhi EDGE
fix walls all wall/srd xlo 0.0 ylo 10.0 units box
fix top all wall/srd zhi v_pressdown

Description:

Bound the simulation with one or more walls which interact with stochastic reaction dynamics (SRD) particles as
slip (smooth) or no-slip (rough) flat surfaces. The wall interaction is actually invoked via the fix srd command,
only on the group of SRD particles it defines, so the group setting for the fix wall/srd command is ignored.

A particle/wall collision occurs if an SRD particle moves outside the wall on a timestep. This alters the position
and velocity of the SRD particle and imparts a force to the wall.

The collision and Tsrd settings specified via the fix srd command affect the SRD/wall collisions. A slip setting for
the collision keyword means that the tangential component of the SRD particle momentum is preserved. Thus
only a normal force is imparted to the wall. The normal component of the new SRD velocity is sampled from a
Gaussian distribution at temperature Tsrd.

For a noslip setting of the collision keyword, both the normal and tangential components of the new SRD velocity
are sampled from a Gaussian distribution at temperature Tsrd. Additionally, a new tangential direction for the
SRD velocity is chosen randomly. This collision style imparts both a normal and tangential force to the wall.

Up to 6 walls or faces can be specified in a single command: xlo, xhi, ylo, yhi, zlo, zhi. A lo face reflects particles
that move to a coordinate less than the wall position, back in the hi direction. A hi face reflects particles that move
to a coordinate higher than the wall position, back in the lo direction.
The position of each wall can be specified in one of 3 ways: as the EDGE of the simulation box, as a constant value, or as a variable. If EDGE is used, then the corresponding boundary of the current simulation box is used. If a numeric constant is specified then the wall is placed at that position in the appropriate dimension (x, y, or z). In both the EDGE and constant cases, the wall will never move. If the wall position is a variable, it should be specified as v_name, where name is an equal-style variable name. In this case the variable is evaluated each timestep and the result becomes the current position of the reflecting wall. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position.

IMPORTANT NOTE: Because the trajectory of the SRD particle is tracked as it collides with the wall, you must insure that r = distance of the particle from the wall, is always > 0 for SRD particles, or LAMMPS will generate an error. This means you cannot start your simulation with SRD particles at the wall position coord (r = 0) or with particles on the wrong side of the wall (r < 0).

IMPORTANT NOTE: If you have 2 or more walls that come together at an edge or corner (e.g. walls in the x and y dimensions), then be sure to set the overlap keyword to yes in the fix srd command, since the walls effectively overlap when SRD particles collide with them. LAMMPS will issue a warning if you do not do this.

IMPORTANT NOTE: The walls of this fix only interact with SRD particles, as defined by the fix srd command. If you are simulating a mixture containing other kinds of particles, then you should typically use another wall command to act on the other particles. Since SRD particles will be colliding both with the walls and the other particles, it is important to insure that the other particle's finite extent does not overlap an SRD wall. If you do not do this, you may generate errors when SRD particles end up “inside” another particle or a wall at the beginning of a collision step.

The units keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant is used. It is not relevant when EDGE or a variable is used to specify a face position.

A box value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A lattice value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacings.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using equal-style variables.

```plaintext
variable ramp equal ramp(0,10)  
fix 1 all wall/srd xlo v_ramp

variable linear equal vdisplace(0,20)  
fix 1 all wall/srd xlo v_linear

variable wiggle equal swiggle(0.0,5.0,3.0)  
fix 1 all wall/srd xlo v_wiggle

variable wiggle equal cwiggle(0.0,5.0,3.0)  
fix 1 all wall/srd xlo v_wiggle
```

The ramp(lo,hi) function adjusts the wall position linearly from lo to hi over the course of a run. The displace(c0,velocity) function does something similar using the equation position = c0 + velocity*delta, where delta is the elapsed time.

The swiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, where omega = 2 PI / period:
position = c0 + A \sin(\omega \delta)

The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

position = c0 + A (1 - \cos(\omega \delta))

**Restart, fix_modify, output, run start/stop, minimize info:**

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global array of values which can be accessed by various output commands. The number of rows in the array is equal to the number of walls defined by the fix. The number of columns is 3, for the x,y,z components of force on each wall.

Note that an outward normal force on a wall will be a negative value for lo walls and a positive value for hi walls. The array values calculated by this fix are "extensive".

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

**Restrictions:**

Any dimension (xyz) that has an SRD wall must be non-periodic.

**Related commands:**

fix srd

**Default:** none
group command

Syntax:

```
group ID style args
```

- **ID** = user-defined name of the group
- **style** = delete or region or type or id or molecule or subtract or union or intersect

```
delete = no args
region args = region-ID
type or id or molecule
  args = one or more atom types, atom IDs, or molecule IDs
  args = logical
    logical = "" or "=" or "==" or "!="
    value = an atom type or atom ID or molecule ID (depending on style)
  args = logical value1 value2
    logical = ""
    value1,value2 = atom types or atom IDs or molecule IDs
      (depending on style)
subtract args = two or more group IDs
union args = one or more group IDs
intersect args = two or more group IDs
```

Examples:

```
group edge region regstrip
group water type 3 4
group sub id <= 150
group polyA molecule  50 250
group boundary subtract all a2 a3
group boundary union lower upper
group boundary intersect upper flow
group boundary delete
```

Description:

Identify a collection of atoms as belonging to a group. The group ID can then be used in other commands such as fix, compute, dump, or velocity to act on those atoms together.

If the group ID already exists, the group command adds the specified atoms to the group.

The delete style removes the named group and un-assigns all atoms that were assigned to that group. Since there is a restriction (see below) that no more than 32 groups can be defined at any time, the delete style allows you to remove groups that are no longer needed, so that more can be specified. You cannot delete a group if it has been used to define a current fix or compute or dump.

The region style puts all atoms in the region volume into the group. Note that this is a static one-time assignment. The atoms remain assigned (or not assigned) to the group even in they later move out of the region volume.

The type, id, and molecule styles put all atoms with the specified atom types, atom IDs, or molecule IDs into the group. These 3 styles can have their arguments specified in one of two formats. The 1st format is a list of values (types or IDs). For example, the 2nd command in the examples above puts all atoms of type 3 or 4 into the group named water. The 2nd format is a logical followed by one or two values (type or ID). The 7 valid logicals are
listed above. All the logicals except take a single argument. The 3rd example above adds all atoms with IDs from 1 to 150 to the group named sub. The logical means "between" and takes 2 arguments. The 4th example above adds all atoms belonging to molecules with IDs from 50 to 250 (inclusive) to the group named polyA.

The subtract style takes a list of two or more existing group names as arguments. All atoms that belong to the 1st group, but not to any of the other groups are added to the specified group.

The union style takes a list of one or more existing group names as arguments. All atoms that belong to any of the listed groups are added to the specified group.

The intersect style takes a list of two or more existing group names as arguments. Atoms that belong to every one of the listed groups are added to the specified group.

A group with the ID all is predefined. All atoms belong to this group. This group cannot be deleted.

Restrictions:

There can be no more than 32 groups defined at one time, including "all".

Related commands:

dump, fix, region, velocity

Default:

All atoms belong to the "all" group.
if command

Syntax:

if boolean then t1 t2 ... elif boolean f1 f2 ... elif boolean f1 f2 ... else e1 e2 ...

- boolean = a Boolean expression evaluated as TRUE or FALSE (see below)
- then = required word
- t1,t2,...,tN = one or more LAMMPS commands to execute if condition is met, each enclosed in quotes
- elif = optional word, can appear multiple times
- f1,f2,...,fN = one or more LAMMPS commands to execute if elif condition is met, each enclosed in quotes (optional arguments)
- else = optional argument
- e1,e2,...,eN = one or more LAMMPS commands to execute if no condition is met, each enclosed in quotes (optional arguments)

Examples:

if "${steps} > 1000" then quit
if "$x <= $y" then "print X is smaller = $x" else "print Y is smaller = $y"
if "(${eng} > 0.0) || ($n <1000)" then &
    "timestep 0.005" &
    elif $n ${eng_previous}" then "jump file1" else "jump file2"

Description:

This command provides an in-then-else capability within an input script. A Boolean expression is evaluated and the result is TRUE or FALSE. Note that as in the examples above, the expression can contain variables, as defined by the variable command, which will be evaluated as part of the expression. Thus a user-defined formula that reflects the current state of the simulation can be used to issue one or more new commands.

If the result of the Boolean expression is TRUE, then one or more commands (t1, t2, ..., tN) are executed. If it is FALSE, then Boolean expressions associated with successive elif keywords are evaluated until one is found to be true, in which case its commands (f1, f2, ..., fN) are executed. If no Boolean expression is TRUE, then the commands associated with the else keyword, namely (e1, e2, ..., eN), are executed. The elif and else keywords and their associated commands are optional. If they aren't specified and the initial Boolean expression is FALSE, then no commands are executed.

The syntax for Boolean expressions is described below.

Each command (t1, f1, e1, etc) can be any valid LAMMPS input script command. If the command is more than one word, it must enclosed in quotes, so it will be treated as a single argument, as in the examples above.

IMPORTANT NOTE: If a command itself requires a quoted argument (e.g. a print command), then double and single quotes can be used and nested in the usual manner, as in the examples above and below. See Section_commands 2 of the manual for more details on using quotes in arguments. Only one level of nesting is allowed, but that should be sufficient for most use cases.

Note that by using the line continuation character "&", the if command can be spread across many lines, though it is still a single command:
if "$a <$b" then &
   "print 'Minimum value = $a'" &
   "run 1000" &
else &
   'print "Minimum value = $b"' &
   "minimize 0.001 0.001 1000 10000"

Note that if one of the commands to execute is quit (of an invalid LAMMPS command such as "blah"), as in the first example above, then executing the command will cause LAMMPS to halt.

Note that by jumping to a label in the same input script, the if command can be used to break out of a loop. See the variable delete command for info on how to delete the associated loop variable, so that it can be re-used later in the input script.

Here is an example of a double loop which uses the if and jump commands to break out of the inner loop when a condition is met, then continues iterating thru the outer loop.

```
label       loopa
variable    a loop 5
label     loopb
variable  b loop 5
print     "A,B = $a,$b"
run       10000
if        '$b > 2' then "print 'Jumping to another script'" "jump in.script break"
next      b
jump      in.script loopb
label       break
variable    b delete
next        a
jump        in.script loopa
```

The Boolean expressions for the if and elif keywords have a C-like syntax. Note that each expression is a single argument within the if command. Thus if you want to include spaces in the expression for clarity, you must enclose the entire expression in quotes.

An expression is built out of numbers:

```
0.2, 100, 1.0e20, -15.4, etc
```

and Boolean operators:

```
```

Each A and B is a number or a variable reference like $a or ${abc}, or another Boolean expression.

If a variable is used it must produce a number when evaluated and substituted for in the expression, else an error will be generated.

Expressions are evaluated left to right and have the usual C-style precedence: the unary logical NOT operator "!" has the highest precedence, the 4 relational operators "", and ">=" are next; the two remaining relational operators "==" and "!=" are next; then the logical AND operator "&&"; and finally the logical OR operator "||" has the lowest precedence. Parenthesis can be used to group one or more portions of an expression and/or enforce a different order of evaluation than what would occur with the default precedence.
The 6 relational operators return either a 1.0 or 0.0 depending on whether the relationship between x and y is TRUE or FALSE. The logical AND operator will return 1.0 if both its arguments are non-zero, else it returns 0.0. The logical OR operator will return 1.0 if either of its arguments is non-zero, else it returns 0.0. The logical NOT operator returns 1.0 if its argument is 0.0, else it returns 0.0.

The overall Boolean expression produces a TRUE result if the result is non-zero. If the result is zero, the expression result is FALSE.

**Restrictions:** none

**Related commands:**

*variable, print*

**Default:** none
improper_style class2 command

improper_style class2/omp command

Syntax:

improper_style class2

Examples:

improper_style class2
improper_coeff 1 100.0 0
improper_coeff * aa 0.0 0.0 0.0 115.06 130.01 115.06

Description:

The class2 improper style uses the potential

\[
E = E_i + E_{aa}
\]

\[
E_i = K \left[ \frac{\chi_{ijkl} + \chi_{kjl} + \chi_{ljik}}{3} - \chi_0 \right]^2
\]

\[
E_{aa} = M_1 (\theta_{ijk} - \theta_1) (\theta_{kjl} - \theta_3) + M_2 (\theta_{ijk} - \theta_1) (\theta_{ijl} - \theta_2) + M_3 (\theta_{ijl} - \theta_2) (\theta_{kjl} - \theta_3)
\]

where \( E_i \) is the improper term and \( E_{aa} \) is an angle-angle term. The 3 X terms in \( E_i \) are an average over 3 out-of-plane angles.

The 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered I,J,K,L. \( X_{IJKL} \) refers to the angle between the plane of I,J,K and the plane of J,K,L, and the bond JK lies in both planes. Similarly for \( X_{KJLI} \) and \( X_{LJIK} \). Note that atom J appears in the common bonds (JI, JK, JL) of all 3 X terms. Thus J (the 2nd atom in the quadruplet) is the atom of symmetry in the 3 X angles.

The subscripts on the various theta’s refer to different combinations of 3 atoms (I,J,K,L) used to form a particular angle. E.g. \( \theta_{IJK} \) is the angle formed by atoms I,J,L with J in the middle. \( \theta_1, \theta_2, \theta_3 \) are the equilibrium positions of those angles. Again, atom J (the 2nd atom in the quadruplet) is the atom of symmetry in the theta angles, since it is always the center atom.

Since atom J is the atom of symmetry, normally the bonds J-I, J-K, J-L would exist for an improper to be defined between the 4 atoms, but this is not required.

See (Sun) for a description of the COMPASS class2 force field.
Coefficients for the Ei and Eaa formulas must be defined for each improper type via the `improper_coeff` command as in the example above, or in the data file or restart files read by the `read_data` or `read_restart` commands.

These are the 2 coefficients for the Ei formula:

- \( K \) (energy/radian^2)
- \( X_0 \) (degrees)

\( X_0 \) is specified in degrees, but LAMMPS converts it to radians internally; hence the units of \( K \) are in energy/radian^2.

For the Eaa formula, each line in a `improper_coeff` command in the input script lists 7 coefficients, the first of which is "aa" to indicate they are AngleAngle coefficients. In a data file, these coefficients should be listed under a "AngleAngle Coeffs" heading and you must leave out the "aa", i.e. only list 6 coefficients after the improper type.

- aa
- M1 (energy/distance)
- M2 (energy/distance)
- M3 (energy/distance)
- \( \theta_1 \) (degrees)
- \( \theta_2 \) (degrees)
- \( \theta_3 \) (degrees)

The \( \theta \) values are specified in degrees, but LAMMPS converts them to radians internally; hence the units of M are in energy/radian^2.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section `accelerate` of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section `accelerate` of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**

This improper style can only be used if LAMMPS was built with the CLASS2 package. See the Making LAMMPS section for more info on packages.

**Related commands:**

`improper_coeff`

**Default:** none
improper_coeff command

Syntax:

improper_coeff N args

- N = improper type (see asterisk form below)
- args = coefficients for one or more improper types

Examples:

improper_coeff 1 300.0 0.0
improper_coeff * 80.2 -1 2
improper_coeff *4 80.2 -1 2

Description:

Specify the improper force field coefficients for one or more improper types. The number and meaning of the coefficients depends on the improper style. Improper coefficients can also be set in the data file read by the read_data command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple improper types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of improper types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using an improper_coeff command can override a previous setting for the same improper type. For example, these commands set the coeffs for all improper types, then overwrite the coeffs for just improper type 2:

improper_coeff * 300.0 0.0
improper_coeff 2 50.0 0.0

A line in a data file that specifies improper coefficients uses the exact same format as the arguments of the improper_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Improper Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

1 300.0 0.0

The improper_style class2 is an exception to this rule, in that an additional argument is used in the input script to allow specification of the cross-term coefficients. See its doc page for details.

Here is an alphabetic list of improper styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated improper_coeff command.

Note that there are also additional improper styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the improper section of this page.
Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

An improper style must be defined before any improper coefficients are set, either in the input script or in a data file.

Related commands:

improper_style

Default: none
improper_style cossq command

improper_style cossq/omp command

Syntax:

improper_style cossq

Examples:

improper_style cossq
improper_coeff 1 4.0 0.0

Description:

The cossq improper style uses the potential

\[ E = \frac{1}{2} K \cos^2 \left( \chi - \chi_0 \right) \]

where \( \chi \) is the improper angle, \( \chi_0 \) is its equilibrium value, and \( K \) is a prefactor.

If the 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered I,J,K,L then \( X \) is the angle between the plane of I,J,K and the plane of J,K,L. Alternatively, you can think of atoms J,K,L as being in a plane, and atom I above the plane, and \( X \) as a measure of how far out-of-plane I is with respect to the other 3 atoms.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- \( K \) (energy/radian^2)
- \( \chi_0 \) (degrees)

\( \chi_0 \) is specified in degrees, but LAMMPS converts it to radians internally; hence the units of \( K \) are in energy/radian^2.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.
You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the
-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input
script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This improper style can only be used if LAMMPS was built with the USER-MISC package. See the Making
LAMMPS section for more info on packages.

Related commands:

improper_coeff

Default: none
improper_style cvff command

improper_style cvff/omp command

Syntax:

improper_style cvff

Examples:

improper_style cvff
improper_coeff 1 80.0 -1 4

Description:

The cvff improper style uses the potential

\[ E = K [1 + d \cos(n\phi)] \]

where \( \phi \) is the improper dihedral angle.

If the 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered I,J,K,L then the improper dihedral angle is between the plane of I,J,K and the plane of J,K,L. Note that because this is effectively a dihedral angle, the formula for this improper style is the same as for dihedral_style harmonic.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- d (+1 or -1)
- n (0,1,2,3,4,6)

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.
See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**

This improper style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

**Related commands:**

improper_coeff

**Default:** none
improper_style harmonic command

improper_style harmonic/omp command

Syntax:

improper_style harmonic

Examples:

improper_style harmonic
improper_coeff 1 100.0 0

Description:

The *harmonic* improper style uses the potential

\[ E = K (\chi - \chi_0)^2 \]

where \( \chi \) is the improper angle, \( \chi_0 \) is its equilibrium value, and \( K \) is a prefactor. Note that the usual \( 1/2 \) factor is included in \( K \).

If the 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered I,J,K,L then \( \chi \) is the angle between the plane of I,J,K and the plane of J,K,L. Alternatively, you can think of atoms J,K,L as being in a plane, and atom I above the plane, and \( \chi \) as a measure of how far out-of-plane I is with respect to the other 3 atoms.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- \( K \) (energy/radian^2)
- \( \chi_0 \) (degrees)

\( \chi_0 \) is specified in degrees, but LAMMPS converts it to radians internally; hence the units of \( K \) are in energy/radian^2.

Styles with a *cuda*, *gpu*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.
You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the 
-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input 
script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This improper style can only be used if LAMMPS was built with the MOLECULAR package (which it is by 
default). See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

Default: none
**improper_style hybrid command**

**Syntax:**

```plaintext
improper_style hybrid style1 style2 ...
```

- `style1,style2 = list of one or more improper styles`

**Examples:**

```plaintext
improper_style hybrid harmonic helix
improper_coeff 1 harmonic 120.0 30
improper_coeff 2 cvff 20.0 -1 2
```

**Description:**

The *hybrid* style enables the use of multiple improper styles in one simulation. An improper style is assigned to each improper type. For example, impropers in a polymer flow (of improper type 1) could be computed with a *harmonic* potential and impropers in the wall boundary (of improper type 2) could be computed with a *cvff* potential. The assignment of improper type to style is made via the `improper_coeff` command or in the data file.

In the `improper_coeff` command, the first coefficient sets the improper style and the remaining coefficients are those appropriate to that style. In the example above, the 2 `improper_coeff` commands would set impropers of improper type 1 to be computed with a *harmonic* potential with coefficients 120.0, 30 for K, X0. Improper type 2 would be computed with a *cvff* potential with coefficients 20.0, -1, 2 for K, d, n.

If the improper *class2* potential is one of the hybrid styles, it requires additional AngleAngle coefficients be specified in the data file. These lines must also have an additional "class2" argument added after the improper type. For improper types which are assigned to other hybrid styles, use the style name (e.g. "harmonic") appropriate to that style. The AngleAngle coefs for that improper type will then be ignored.

An improper style of *none* can be specified as the 2nd argument to the `improper_coeff` command, if you desire to turn off certain improper types.

**Restrictions:**

This improper style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

Unlike other improper styles, the hybrid improper style does not store improper coefficient info for individual sub-styles in a binary restart files. Thus when restarting a simulation from a restart file, you need to re-specify improper_coeff commands.

**Related commands:**

`improper_coeff`

**Default:** none
improper_style none command

Syntax:

improper_style none

Examples:

improper_style none

Description:

Using an improper style of none means improper forces are not computed, even if quadruplets of improper atoms were listed in the data file read by the read_data command.

Restrictions: none

Related commands: none

Default: none
improper_style ring command

improper_style ring/omp command

Syntax:

improper_style ring

Examples:

improper_style ring
improper_coeff 1 8000 70.5

Description:

The *ring* improper style uses the potential

\[
E = \frac{1}{6} K \left( \Delta_{ijl} + \Delta_{ijk} + \Delta_{kjl} \right)^6
\]

\[
\Delta_{ijl} = \cos \theta_{ijl} - \cos \theta_0
\]

\[
\Delta_{ijk} = \cos \theta_{ijk} - \cos \theta_0
\]

\[
\Delta_{kjl} = \cos \theta_{kjl} - \cos \theta_0
\]

where K is a prefactor, theta is the angle formed by the atoms specified by (i,j,k,l) indices and theta0 its equilibrium value.

If the 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered i,j,k,l then theta_{ijl} is the angle between atoms i,j and l, theta_{ijk} is the angle between atoms i,j and k, theta_{kjl} is the angle between atoms j,k, and l.

The "ring" improper style implements the improper potential introduced by Destree et al., in Equation (9) of (Destree). This potential does not affect small amplitude vibrations but is used in an ad-hoc way to prevent the onset of accidentally large amplitude fluctuations leading to the occurrence of a planar conformation of the three bonds i-j, j-k and j-l, an intermediate conformation toward the chiral inversion of a methine carbon. In the "Impropers" section of data file four atoms: i, j, k and l are specified with i,j and l lying on the backbone of the chain and k specifying the chirality of j.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/radian^2)
- theta0 (degrees)
theta0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This improper style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

improper_style command

Syntax:

improper_style style

- style = none or hybrid or class2 or cvff or harmonic

Examples:

improper_style harmonic
improper_style cvff
improper_style hybrid cvff harmonic

Description:

Set the formula(s) LAMMPS uses to compute improper interactions between quadruplets of atoms, which remain in force for the duration of the simulation. The list of improper quadruplets is read in by a read_data or read_restart command from a data or restart file. Note that the ordering of the 4 atoms in an improper quadruplet determines the definition of the improper angle used in the formula for each style. See the doc pages of individual styles for details.

Hybrid models where impropers are computed using different improper potentials can be setup using the hybrid improper style.

The coefficients associated with an improper style can be specified in a data or restart file or via the improper_coeff command.

All improper potentials store their coefficient data in binary restart files which means improper_style and improper_coeff commands do not need to be re-specified in an input script that restarts a simulation. See the read_restart command for details on how to do this. The one exception is that improper_style hybrid only stores the list of sub-styles in the restart file; improper coefficients need to be re-specified.

IMPORTANT NOTE: When both an improper and pair style is defined, the special_bonds command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between a group of 4 bonded atoms.

Here is an alphabetic list of improper styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated improper_coeff command.

Note that there are also additional improper styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the improper section of this page.

- improper_style none - turn off improper interactions
- improper_style hybrid - define multiple styles of improper interactions
- improper_style class2 - COMPASS (class 2) improper
- improper_style cvff - CVFF improper
- improper_style harmonic - harmonic improper
- improper_style umbrella - DREIDING improper
Restrictions:

Improper styles can only be set for atom_style choices that allow impropers to be defined.

Most improper styles are part of the MOLECULAR package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual improper potentials tell if it is part of a package.

Related commands:

improper_coeff

Default:

improper_style none
improper_style umbrella command

improper_style umbrella/omp command

Syntax:

improper_style umbrella

Examples:

improper_style umbrella
improper_coeff 1 100.0 180.0

Description:

The umbrella improper style uses the following potential, which is commonly referred to as a classic inversion and used in the DREIDING force field:

\[ E = \frac{1}{2} K \left( \frac{1 + \cos \omega_0}{\sin \omega_0} \right)^2 (\cos \omega - \cos \omega_0) \quad \omega_0 \neq 0^\circ \]

\[ E = K (1 - \cos \omega) \quad \omega_0 = 0^\circ \]

where K is the force constant and omega is the angle between the IL axis and the IJK plane:

If omega0 = 0 the potential term has a minimum for the planar structure. Otherwise it has two minima at +/- omega0, with a barrier in between.

See (Mayo) for a description of the DREIDING force field.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:
• K (energy)
• omega0 (degrees)

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix command-line switch` when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**

This improper style can only be used if LAMMPS was built with the MOLECULAR package (which it is by default). See the Making LAMMPS section for more info on packages.

**Related commands:**

`improper_coeff`

**Default:** none

include command

Syntax:

include file

- file = filename of new input script to switch to

Examples:

include newfile
include in.run2

Description:

This command opens a new input script file and begins reading LAMMPS commands from that file. When the new file is finished, the original file is returned to. Include files can be nested as deeply as desired. If input script A includes script B, and B includes A, then LAMMPS could run for a long time.

If the filename is a variable (see the variable command), different processor partitions can run different input scripts.

Restrictions: none

Related commands:

variable, jump

Default: none
jump command

Syntax:

```
jump file label
```

- file = filename of new input script to switch to
- label = optional label within file to jump to

Examples:

```
jump newfile
jump in.run2 runloop
jump SELF runloop
```

Description:

This command closes the current input script file, opens the file with the specified name, and begins reading LAMMPS commands from that file. Unlike the include command, the original file is not returned to, although by using multiple jump commands it is possible to chain from file to file or back to the original file.

If the word "SELF" is used for the filename, then the current input script is re-opened and read again.

IMPORTANT NOTE: The SELF option is not guaranteed to work when the current input script is being read through stdin (standard input), e.g.

```
lmp_g++ <in.script
```

since the SELF option invokes the C-library rewind() call, which may not be supported for stdin on some systems. This can be worked around by using the -in command-line argument or the -var command-line argument to pass the script name as a variable to the input script. In the latter case, the "fname" variable could be used in place of SELF. E.g.

```
lmp_g++ -in in.script
```

```
lmp_g++ -var fname n.script <in.script
```

The 2nd argument to the jump command is optional. If specified, it is treated as a label and the new file is scanned (without executing commands) until the label is found, and commands are executed from that point forward. This can be used to loop over a portion of the input script, as in this example. These commands perform 10 runs, each of 10000 steps, and create 10 dump files named file.1, file.2, etc. The next command is used to exit the loop after 10 iterations. When the "a" variable has been incremented for the tenth time, it will cause the next jump command to be skipped.

```
variable a loop 10
label loop
dump 1 all atom 100 file.$a
run 10000
undump 1
next a
jump in.lj loop
```
If the `jump file` argument is a variable, the `jump` command can be used to cause different processor partitions to run different input scripts. In this example, LAMMPS is run on 40 processors, with 4 partitions of 10 procs each. An in.file containing the example variable and jump command will cause each partition to run a different simulation.

```
mpirun -np 40 lmp_ibm -partition 4x10 -in in.file
variable f world script.1 script.2 script.3 script.4
jump $f
```

Here is an example of a double loop which uses the `if` and `jump` commands to break out of the inner loop when a condition is met, then continues iterating thru the outer loop.

```plaintext
label       loopa
variable    a loop 5
label       loopb
variable    b loop 5
print       "A,B = $a,$b"
run         10000
if          $b > 2 then "jump in.script break"
next        b
jump         in.script loopb
label       break
variable    b delete
next         a
jump         in.script loopa
```

**Restrictions:**

If you jump to a file and it does not contain the specified label, LAMMPS will come to the end of the file and exit.

**Related commands:**

variable, include, label, next

**Default:** none
kspace_modify command

Syntax:

kspace_modify keyword value ...

- one or more keyword/value pairs may be listed
- keyword = mesh or order or gewald or slab or (nozforce or compute or diff)

  mesh value = x y z  
  x,y,z = PPPM FFT grid size in each dimension

  order value = N  
  N = grid extent of Gaussian for PPPM mapping of each charge

  force value = accuracy (force units)

  gewald value = rinv (1/distance units) 
  rinv = PPPM G-ewald parameter

  slab value = volfactor or nozforce
  volfactor = ratio of the total extended volume used in the 
  2d approximation compared with the volume of the simulation domain

  nozforce turns off kspace forces in the z direction

  compute value = yes or no

  diff value = ik or ad

Examples:

kspace_modify mesh 24 24 30 order 6
kspace_modify slab 3.0

Description:

Set parameters used by the kspace solvers defined by the kspace_style command. Not all parameters are relevant to all kspace styles.

The mesh keyword sets the 3d FFT grid size for kspace style ppm. Each dimension must be factorizable into powers of 2, 3, and 5. When this option is not set, the PPPM solver chooses its own grid size, consistent with the user-specified accuracy and pairwise cutoff. Values for x,y,z of 0,0,0 unset the option.

The order keyword determines how many grid spacings an atom's charge extends when it is mapped to the FFT grid in kspace style ppm. The default for this parameter is 5, which means each charge spans 5 grid cells in each dimension. The minimum allowed setting is 2 and the maximum allowed setting is 7. The larger the value of this parameter, the smaller the FFT grid will need to be to achieve the requested precision. Conversely, the smaller the order value, the larger the grid will be. Note that there is an inherent trade-off involved: a small grid will lower the cost of FFTs, but a large order parameter will increase the cost of interpolating charge/fields to/from the grid. And vice versa.

The order parameter may be reset by LAMMPS when it sets up the PPPM FFT grid if the implied grid stencil extends beyond the grid cells owned by neighboring processors. Typically this will only occur when small problems are run on large numbers of processors. A warning will be generated indicating the order parameter is being reduced to allow LAMMPS to run the problem.

The force keyword overrides the relative accuracy parameter set by the kspace_style command with an absolute accuracy. The accuracy determines the RMS error in per-atom forces calculated by the long-range solver and is thus specified in force units. A negative value for the accuracy setting means to use the relative accuracy...
parameter. The accuracy setting is used in conjunction with the pairwise cutoff to determine the number of K-space vectors for style ewald or the FFT grid size for style pppm.

The gewald keyword sets the value of the Ewald or PPPM G-ewald parameter as \( r_{\text{inv}} \) in reciprocal distance units. Without this setting, LAMMPS chooses the parameter automatically as a function of cutoff, precision, grid spacing, etc. This means it can vary from one simulation to the next which may not be desirable for matching a KSpace solver to a pre-tabulated pairwise potential. This setting can also be useful if Ewald or PPPM fails to choose a good grid spacing and G-ewald parameter automatically. If the value is set to 0.0, LAMMPS will choose the G-ewald parameter automatically.

The slab keyword allows an Ewald or PPPM solver to be used for a systems that are periodic in x,y but non-periodic in z - a boundary setting of "boundary p p f". This is done by treating the system as if it were periodic in z, but inserting empty volume between atom slabs and removing dipole inter-slab interactions so that slab-slab interactions are effectively turned off. The volfactor value sets the ratio of the extended dimension in z divided by the actual dimension in z. The recommended value is 3.0. A larger value is inefficient; a smaller value introduces unwanted slab-slab interactions. The use of fixed boundaries in z means that the user must prevent particle migration beyond the initial z-bounds, typically by providing a wall-style fix. The methodology behind the slab option is explained in the paper by (Yeh). An alternative slab option can be invoked with the nozforce keyword in lieu of the volfactor. This turns off all kspace forces in the z direction.

The compute keyword allows Kspace computations to be turned off, even though a kspace_style is defined. This is not useful for running a real simulation, but can be useful for debugging purposes or for computing only partial forces that do not include the Kspace contribution. You can also do this by simply not defining a kspace_style, but a Kspace-compatible pair_style requires a kspace_style to be defined. This keyword gives you that option.

The diff keyword specifies the differentiation scheme used by the PPPM method to compute forces on particles given electrostatic potentials on the PPPM mesh. The ik approach is the default. It performs differentiation in Kspace, but uses 3 FFTs to transfer the computed fields back to real space (total of 4 FFTs per timestep). The analytic differentiation, or ad approach uses only 1 FFT to transfer the computed fields back to real space (total of 2 FFTs per timestep), but requires a somewhat larger PPPM mesh to achieve the same accuracy as the ik approach.

IMPORTANT NOTE: Currently, only the pppm style supports the ad option. Support from other pppm variants will be added later.

IMPORTANT NOTE: If you run the ad option with a constant pressure simulation (e.g. with fix npt), you may see a net slow-down. This is because the ad option requires more expensive pre-computation whenever the box size changes. This happens every step for constant-pressure simulations.

Restrictions: none

Related commands:

kspace_style, boundary

Default:

The option defaults are mesh = 0 0 0, order = 5, force = -1.0, gewald = 0.0, slab = 1.0, compute = yes, and diff = ik.

(Yeh) Yeh and Berkowitz, J Chem Phys, 111, 3155 (1999).
kspace_style command

Syntax:

    kspace_style style value

- style = none or ewald or ewald/omp or ewald/n or pppm or pppm/cg or pppm/tip4p or pppm/gpu or pppm/omp or pppm/cg/omp or pppm/tip4p/omp or pppm/proxy or pppm/tip4p/proxy

  none value = none
  ewald value = accuracy
  ewald/omp value = accuracy
  ewald/n value = accuracy
  pppm value = accuracy
  pppm/cg value = accuracy (smallq)
  pppm/cg/omp value = accuracy
  pppm/tip4p value = accuracy
  pppm/tip4p/omp value = accuracy
  pppm/gpu value = accuracy
  pppm/omp value = accuracy
  pppm/tip4p/omp value = accuracy
  pppm/proxy value = accuracy
  pppm/tip4p/proxy value = accuracy

Examples:

    kspace_style pppm 1.0e-4
    kspace_style pppm/cg 1.0e-5 1.0e-6
    kspace_style none

Description:

Define a K-space solver for LAMMPS to use each timestep to compute long-range Coulombic interactions or long-range 1/r^N interactions. When such a solver is used in conjunction with an appropriate pair style, the cutoff for Coulombic or other 1/r^N interactions is effectively infinite; each charge in the system interacts with charges in an infinite array of periodic images of the simulation domain.

The ewald style performs a standard Ewald summation as described in any solid-state physics text.

The ewald/n style augments ewald by adding long-range dispersion sum capabilities for 1/r^N potentials and is useful for simulation of interfaces (Veld). It also performs standard coulombic Ewald summations, but in a more efficient manner than the ewald style. The 1/r^N capability means that Lennard-Jones or Buckingham potentials can be used with ewald/n without a cutoff, i.e. they become full long-range potentials.

Currently, only the ewald/n style can be used with non-orthogonal (triclinic symmetry) simulation boxes.
The `pppm` style invokes a particle-particle particle-mesh solver (Hockney) which maps atom charge to a 3d mesh, uses 3d FFTs to solve Poisson's equation on the mesh, then interpolates electric fields on the mesh points back to the atoms. It is closely related to the particle-mesh Ewald technique (PME) (Darden) used in AMBER and CHARMM. The cost of traditional Ewald summation scales as \(N^{3/2}\) where \(N\) is the number of atoms in the system. The PPPM solver scales as \(N\log(N)\) due to the FFTs, so it is almost always a faster choice (Pollock).

The `pppm/cg` style is identical to the `pppm` style except that it has an optimization for systems where most particles are uncharged. The optional `smallq` argument defines the cutoff for the absolute charge value which determines whether a particle is considered charged or not. Its default value is 1.0e-5.

The `pppm/tip4p` style is identical to the `pppm` style except that it adds a charge at the massless 4th site in each TIP4P water molecule. It should be used with pair styles with a `long/tip4p` in their style name.

The `pppm/proxy` style is a special variant for calculations in hybrid OpenMP/MPI parallel mode. It is functionally equivalent with `pppm`, but it its force computation is being executed as a single thread concurrently with a multi-threaded non-bonded calculation for a pair style with `pppm/omp` suffix. For calculations across many multi-core nodes, this can have a performance benefit over performing the real and reciprocal space part separately, specifically when otherwise the time spent on the pair style would slightly less than in `pppm` without threading.

Note that the PPPM styles can be used with single-precision FFTs by using the compiler switch -DFFT_SINGLE for the FFT_INC setting in your lo-level Makefile. This setting also changes some of the PPPM operations (e.g. mapping charge to mesh and interpolating electric fields to particles) to be performed in single precision. This option can speed-up long-range calculations, particularly in parallel or on GPUs. The use of the -DFFT_SINGLE flag is discussed in this section of the manual.

When a kspace style is used, a pair style that includes the short-range correction to the pairwise Coulombic or other \(1/r^N\) forces must also be selected. For Coulombic interactions, these styles are ones that have a `coul/long` in their style name. For \(1/r^6\) dispersion forces in a Lennard-Jones or Buckingham potential, see the pair_style `lj/coul` or `pair_style buck/coul` commands.

The specified accuracy determines the relative RMS error in per-atom forces calculated by the long-range solver. It is set as a dimensionless number, relative to the force that two unit point charges (e.g. 2 monovalent ions) exert on each other at a distance of 1 Angstrom. This reference value was chosen as representative of the magnitude of electrostatic forces in atomic systems. Thus an accuracy value of 1.0e-4 means that the RMS error will be a factor of 10000 smaller than the reference force.

The accuracy setting is used in conjunction with the pairwise cutoff to determine the number of K-space vectors for style `ewald` or the FFT grid size for style `pppm`.

RMS force errors in real space for `ewald` and `pppm` are estimated using equation 18 of (Kolafa), which is also referenced as equation 9 of (Petersen). RMS force errors in K-space for `ewald` are estimated using equation 11 of (Petersen), which is similar to equation 32 of (Kolafa). RMS force errors in K-space for `pppm` are estimated using equation 38 of (Deserno).

See the `kspace_modify` command for additional options of the K-space solvers that can be set, including a `force` option for setting an absolute RMS error in forces, as opposed to a relative RMS error.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for
round-off and precision issues.

More specifically, the `pppm/gpu` style performs charge assignment and force interpolation calculations on the GPU. These processes are performed either in single or double precision, depending on whether the `-DFFT_SINGLE` setting was specified in your lo-level Makefile, as discussed above. The FFTs themselves are still calculated on the CPU. If `pppm/gpu` is used with a GPU-enabled pair style, part of the PPPM calculation can be performed concurrently on the GPU while other calculations for non-bonded and bonded force calculation are performed on the CPU.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP, and OPT packages respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Restrictions:**

A simulation must be 3d and periodic in all dimensions to use an Ewald or PPPM solver. The only exception is if the slab option is set with `kspace_modify`, in which case the xy dimensions must be periodic and the z dimension must be non-periodic.

Kspace styles are part of the KSPACE package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The `ewald/n` style is part of the USER-EWALDN package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

When using a long-range pairwise TIP4P potential, you must use kspace style `pppm/tip4p` and vice versa.

**Related commands:**

`kspace_modify`, `pair_style lj/cut/coul/long`, `pair_style lj/charmm/coul/long`, `pair_style lj/coul`, `pair_style buck/coul/long`

**Default:**

`kspace_style none`


label command

Syntax:

label ID

- ID = string used as label name

Examples:

label xyz
label loop

Description:

Label this line of the input script with the chosen ID. Unless a jump command was used previously, this does nothing. But if a jump command was used with a label argument to begin invoking this script file, then all command lines in the script prior to this line will be ignored. I.e. execution of the script will begin at this line. This is useful for looping over a section of the input script as discussed in the jump command.

Restrictions: none

Related commands: none

Default: none
lattice command

Syntax:

lattice style scale keyword values ...

- **style** = *none* or *sc* or *bcc* or *fcc* or *hcp* or *diamond* or *sq* or *sq2* or *hex* or *custom*
- **scale** = scale factor between lattice and simulation box

  - for style *none*:
    - scale is not specified (nor any optional arguments)
  - for all other styles:
    - scale = reduced density rho* (for LJ units)
    - scale = lattice constant in distance units (for non-LJ units)

- **zero** or more keyword/value pairs may be appended
- **keyword** = *origin* or *orient* or *spacing* or *a1* or *a2* or *a3* or *basis*

  - **origin** values = x y z
    - x,y,z = fractions of a unit cell (0 <= x,y,z <1)
  - **orient** values = dim i j k
    - dim = x or y or z
    - i,j,k = integer lattice directions
  - **spacing** values = dx dy dz
    - dx,dy,dz = lattice spacings in the x,y,z box directions
  - **a1,a2,a3** values = x y z
    - x,y,z = primitive vector components that define unit cell
  - **basis** values = x y z
    - x,y,z = fractional coords of a basis atom (0 <= x,y,z <1)

Examples:

lattice fcc 3.52
lattice hex 0.85
lattice sq 0.8 origin 0.0 0.5 0.0 orient x 1 1 0 orient y -1 1 0
lattice custom 3.52 a1 1.0 0.0 0.0 a2 0.5 1.0 0.0 a3 0.0 0.0 0.5 &
  basis 0.0 0.0 0.0 basis 0.5 0.5 0.5
lattice none

Description:

Define a lattice for use by other commands. In LAMMPS, a lattice is simply a set of points in space, determined by a unit cell with basis atoms, that is replicated infinitely in all dimensions. The arguments of the lattice command can be used to define a wide variety of crystallographic lattices.

A lattice is used by LAMMPS in two ways. First, the create_atoms command creates atoms on the lattice points inside the simulation box. Note that the create_atoms command allows different atom types to be assigned to different basis atoms of the lattice. Second, the lattice spacing in the x,y,z dimensions implied by the lattice, can be used by other commands as distance units (e.g. create_box, region and velocity), which are often convenient to use when the underlying problem geometry is atoms on a lattice.

The lattice style must be consistent with the dimension of the simulation - see the dimension command. Styles *sc* or *bcc* or *fcc* or *hcp* or *diamond* are for 3d problems. Styles *sq* or *sq2* or *hex* are for 2d problems. Style *custom* can be used for either 2d or 3d problems.
A lattice consists of a unit cell, a set of basis atoms within that cell, and a set of transformation parameters (scale, origin, orient) that map the unit cell into the simulation box. The vectors $a_1, a_2, a_3$ are the edge vectors of the unit cell. This is the nomenclature for "primitive" vectors in solid-state crystallography, but in LAMMPS the unit cell they determine does not have to be a "primitive cell" of minimum volume.

Lattices of style $sc$, $fcc$, $bcc$, and $diamond$ are 3d lattices that define a cubic unit cell with edge length = 1.0. This means $a_1 = 1 0 0$, $a_2 = 0 1 0$, and $a_3 = 0 0 1$. Style $hcp$ has $a_1 = 1 0 0$, $a_2 = 0 \sqrt{3} 0$, and $a_3 = 0 0 \sqrt{8/3}$. The placement of the basis atoms within the unit cell are described in any solid-state physics text. A $sc$ lattice has 1 basis atom at the lower-left-bottom corner of the cube. A $bcc$ lattice has 2 basis atoms, one at the corner and one at the center of the cube. A $fcc$ lattice has 4 basis atoms, one at the corner and 3 at the cube face centers. A $hcp$ lattice has 4 basis atoms, two in the $z = 0$ plane and 2 in the $z = 0.5$ plane. A $diamond$ lattice has 8 basis atoms.

Lattices of style $sq$ and $sq2$ are 2d lattices that define a square unit cell with edge length = 1.0. This means $a_1 = 1 0 0$ and $a_2 = 0 1 0$. A $sq$ lattice has 1 basis atom at the lower-left corner of the square. A $sq2$ lattice has 2 basis atoms, one at the corner and one at the center of the square. A $hex$ style is also a 2d lattice, but the unit cell is rectangular, with $a_1 = 1 0 0$ and $a_2 = 0 \sqrt{3} 0$. It has 2 basis atoms, one at the corner and one at the center of the rectangle.

A lattice of style $custom$ allows you to specify $a_1$, $a_2$, $a_3$, and a list of basis atoms to put in the unit cell. By default, $a_1$ and $a_2$ and $a_3$ are 3 orthogonal unit vectors (edges of a unit cube). But you can specify them to be of any length and non-orthogonal to each other, so that they describe a tilted parallelepiped. Via the basis keyword you add atoms, one at a time, to the unit cell. Its arguments are fractional coordinates ($0.0 \leq x,y,z < 1.0$), so that a value of 0.5 means a position half-way across the unit cell in that dimension.

This sub-section discusses the arguments that determine how the idealized unit cell is transformed into a lattice of points within the simulation box.

The scale argument determines how the size of the unit cell will be scaled when mapping it into the simulation box. I.e. it determines a multiplicative factor to apply to the unit cell, to convert it to a lattice of the desired size and distance units in the simulation box. The meaning of the scale argument depends on the units being used in your simulation.

For all unit styles except $lj$, the scale argument is specified in the distance units defined by the unit style. For example, in real or metal units, if the unit cell is a unit cube with edge length 1.0, specifying scale = 3.52 would create a cubic lattice with a spacing of 3.52 Angstroms. In cgs units, the spacing would be 3.52 cm.

For unit style $lj$, the scale argument is the Lennard-Jones reduced density, typically written as $\rho^*$. LAMMPS converts this value into the multiplicative factor via the formula "$factor^{dim} = \rho/\rho^*$", where $\rho = N/V$ with $V =$ the volume of the lattice unit cell and $N =$ the number of basis atoms in the unit cell (described below), and dim = 2 or 3 for the dimensionality of the simulation. Effectively, this means that if LJ particles of size sigma = 1.0 are used in the simulation, the lattice of particles will be at the desired reduced density.

The origin option specifies how the unit cell will be shifted or translated when mapping it into the simulation box. The x,y,z values are fractional values ($0.0 \leq x,y,z < 1.0$) meaning shift the lattice by a fraction of the lattice spacing in each dimension. The meaning of "lattice spacing" is discussed below.

The orient option specifies how the unit cell will be rotated when mapping it into the simulation box. The dim argument is one of the 3 coordinate axes in the simulation box. The other 3 arguments are the crystallographic direction in the lattice that you want to orient along that axis, specified as integers. E.g. "orient x 2 1 0" means the x-axis in the simulation box will be the [210] lattice direction. The 3 lattice directions you specify must be mutually orthogonal and obey the right-hand rule, i.e. (X cross Y) points in the Z direction. Note that this description is really only valid for orthogonal lattices. If you are using the more general lattice style $custom$ with
non-orthogonal $a_1,a_2,a_3$ vectors, then think of the 3 \textit{orient} options as creating a 3x3 rotation matrix which is applied to $a_1,a_2,a_3$ to rotate the original unit cell to a new orientation in the simulation box.

Several LAMMPS commands have the option to use distance units that are inferred from "lattice spacing" in the \textit{x,y,z} box directions. E.g. the \texttt{region} command can create a block of size 10x20x20, where 10 means 10 lattice spacings in the \textit{x} direction.

The \textit{spacing} option sets the 3 lattice spacings directly. All must be non-zero (use 1.0 for \textit{dz} in a 2d simulation). The specified values are multiplied by the multiplicative factor described above that is associated with the scale factor. Thus a spacing of 1.0 means one unit cell independent of the scale factor. This option can be useful if the spacings LAMMPS computes are inconvenient to use in subsequent commands, which can be the case for non-orthogonal or rotated lattices.

If the \textit{spacing} option is not specified, the lattice spacings are computed by LAMMPS in the following way. A unit cell of the lattice is mapped into the simulation box (scaled, shifted, rotated), so that it now has (perhaps) a modified size and orientation. The lattice spacing in \textit{x} is defined as the difference between the min/max extent of the \textit{x} coordinates of the 8 corner points of the modified unit cell. Similarly, the \textit{y} and \textit{z} lattice spacings are defined as the difference in the min/max of the \textit{y} and \textit{z} coordinates.

Note that if the unit cell is orthogonal with axis-aligned edges (not rotated via the \textit{orient} keyword), then the lattice spacings in each dimension are simply the scale factor (described above) multiplied by the length of $a_1,a_2,a_3$. Thus a \textit{hex} style lattice with a scale factor of 3.0 Angstroms, would have a lattice spacing of 3.0 in \textit{x} and $3*\sqrt{3.0}$ in \textit{y}.

IMPORTANT NOTE: For non-orthogonal unit cells and/or when a rotation is applied via the \textit{orient} keyword, then the lattice spacings may be less intuitive. In particular, in these cases, there is no guarantee that the lattice spacing is an integer multiple of the periodicity of the lattice in that direction. Thus, if you create an orthogonal periodic simulation box whose size in a dimension is a multiple of the lattice spacing, and then fill it with atoms via the \texttt{create\_atoms} command, you will NOT necessarily create a periodic system. I.e. atoms may overlap incorrectly at the faces of the simulation box.

Regardless of these issues, the values of the lattice spacings LAMMPS calculates are printed out, so their effect in commands that use the spacings should be decipherable.

The command "lattice none" can be used to turn off a previous lattice definition. Any command that attempts to use the lattice directly (\texttt{create\_atoms}) or associated lattice spacings will then generate an error. No additional arguments need be used with "lattice none".

Restrictions:

The $a_1,a_2,a_3,basis$ keywords can only be used with style \textit{custom}.

Related commands:

\texttt{dimension}, \texttt{create\_atoms}, \texttt{region}

Default:

\texttt{lattice none}

For other lattice styles, the option defaults are origin = 0.0 0.0 0.0, orient = x 1 0 0, orient = y 0 1 0, orient = z 0 0 1, $a_1 = 1\ 0\ 0$, $a_2 = 0\ 1\ 0$, and $a_3 = 0\ 0\ 1$. 

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log command

Syntax:

log file

  • file = name of new logfile

Examples:

log log.equil

Description:

This command closes the current LAMMPS log file, opens a new file with the specified name, and begins logging information to it. If the specified file name is *none*, then no new log file is opened.

If multiple processor partitions are being used, the file name should be a variable, so that different processors do not attempt to write to the same log file.

The file "log.lammps" is the default log file for a LAMMPS run. The name of the initial log file can also be set by the command-line switch -log. See Section_6 for details.

Restrictions: none

Related commands: none

Default:

The default LAMMPS log file is named log.lammps
mass command

Syntax:

mass I value

- I = atom type (see asterisk form below)
- value = mass

Examples:

mass 1 1.0
mass * 62.5
mass 2* 62.5

Description:

Set the mass for all atoms of one or more atom types. Per-type mass values can also be set in the read_data data file using the "Masses" keyword. See the units command for what mass units to use.

The I index can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the mass for multiple atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

A line in a data file that follows the "Masses" keyword specifies mass using the same format as the arguments of the mass command in an input script, except that no wild-card asterisk can be used. For example, under the "Masses" section of a data file, the line that corresponds to the 1st example above would be listed as

1 1.0

Note that the mass command can only be used if the atom style requires per-type atom mass to be set. Currently, all but the sphere and ellipsoid and peri styles do. They require mass to be set for individual particles, not types. Per-atom masses are defined in the data file read by the read_data command, or set to default values by the create_atoms command. Per-atom masses can also be set to new values by the set mass or set density commands.

Also note that pair_style eam defines the masses of atom types in the EAM potential file, in which case the mass command is normally not used.

If you define a hybrid atom style which includes one (or more) sub-styles which require per-type mass and one (or more) sub-styles which require per-atom mass, then you must define both. However, in this case the per-type mass will be ignored; only the per-atom mass will be used by LAMMPS.

Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

All masses must be defined before a simulation is run. They must also all be defined before a velocity or fix shake command is used.
The mass assigned to any type or atom must be > 0.0.

**Related commands:** none

**Default:** none
min_modify command

Syntax:

min_modify keyword values ...

• one or more keyword/value pairs may be listed

    keyword = dmax or line
    dmax value = max
    max = maximum distance for line search to move (distance units)
    line value = backtrack or quadratic or forcezero
    backtrack,quadratic,forcezero = style of linesearch to use

Examples:

min_modify dmax 0.2

Description:

This command sets parameters that affect the energy minimization algorithms selected by the min_style command. The various settings may affect the convergence rate and overall number of force evaluations required by a minimization, so users can experiment with these parameters to tune their minimizations.

The cg and sd minimization styles have an outer iteration and an inner iteration which is steps along a one-dimensional line search in a particular search direction. The dmax parameter is how far any atom can move in a single line search in any dimension (x, y, or z). For the quickmin and fire minimization styles, the dmax setting is how far any atom can move in a single iteration (timestep). Thus a value of 0.1 in real units means no atom will move further than 0.1 Angstroms in a single outer iteration. This prevents highly overlapped atoms from being moved long distances (e.g. through another atom) due to large forces.

The choice of line search algorithm for the cg and sd minimization styles can be selected via the line keyword. The default backtracking search is robust and should always find a local energy minimum. However, it will "converge" when it can no longer reduce the energy of the system. Individual atom forces may still be larger than desired at this point, because the energy change is measured as the difference of two large values (energy before and energy after) and that difference may be smaller than machine epsilon even if atoms could move in the gradient direction to reduce forces further.

By contrast, the quadratic line search algorithm tries to reduce the forces to zero, while guaranteeing that the energy changes is not positive (uphill). For some systems, it may also be more efficient than the backtracking algorithm by requiring fewer energy/force evaluations. The forcezero line search algorithm is similar to quadratic. It may be more efficient than quadratic on some systems.

Restrictions: none

Related commands:

min_style, minimize

Default:
The option defaults are $d_{\text{max}} = 0.1$ and line = backtrack.
**min_style command**

**Syntax:**

```plaintext
min_style style
```

- `style = cg` or `hftn` or `sd` or `quickmin` or `fire`

**Examples:**

```plaintext
min_style cg
min_style fire
```

**Description:**

Choose a minimization algorithm to use when a `minimize` command is performed.

Style *cg* is the Polak-Ribiere version of the conjugate gradient (CG) algorithm. At each iteration the force gradient is combined with the previous iteration information to compute a new search direction perpendicular (conjugate) to the previous search direction. The PR variant affects how the direction is chosen and how the CG method is restarted when it ceases to make progress. The PR variant is thought to be the most effective CG choice for most problems.

Style *hftn* is a Hessian-free truncated Newton algorithm. At each iteration a quadratic model of the energy potential is solved by a conjugate gradient inner iteration. The Hessian (second derivatives) of the energy is not formed directly, but approximated in each conjugate search direction by a finite difference directional derivative. When close to an energy minimum, the algorithm behaves like a Newton method and exhibits a quadratic convergence rate to high accuracy. In most cases the behavior of *hftn* is similar to *cg*, but it offers an alternative if *cg* seems to perform poorly. This style is not affected by the `min_modify` command.

Style *sd* is a steepest descent algorithm. At each iteration, the search direction is set to the downhill direction corresponding to the force vector (negative gradient of energy). Typically, steepest descent will not converge as quickly as CG, but may be more robust in some situations.

Style *quickmin* is a damped dynamics method described in (Sheppard), where the damping parameter is related to the projection of the velocity vector along the current force vector for each atom. The velocity of each atom is initialized to 0.0 by this style, at the beginning of a minimization.

Style *fire* is a damped dynamics method described in (Bitzek), which is similar to *quickmin* but adds a variable timestep and alters the projection operation to maintain components of the velocity non-parallel to the current force vector. The velocity of each atom is initialized to 0.0 by this style, at the beginning of a minimization.

Either the *quickmin* and *fire* styles are useful in the context of nudged elastic band (NEB) calculations via the `neb` command.

**IMPORTANT NOTE:** The *quickmin* and *fire* styles do not yet support the use of the `fix box/relax` command or minimizations involving the electron radius in eFF models.

**Restrictions:** none
Related commands:

\texttt{min_modify, minimize, neb}

Default:

\texttt{min_style cg}


minimize command

Syntax:

minimize etol ftol maxiter maxeval

- etol = stopping tolerance for energy (unitless)
- ftol = stopping tolerance for force (force units)
- maxiter = max iterations of minimizer
- maxeval = max number of force/energy evaluations

Examples:

minimize 1.0e-4 1.0e-6 100 1000
minimize 0.0 1.0e-8 1000 100000

Description:

Perform an energy minimization of the system, by iteratively adjusting atom coordinates. Iterations are terminated when one of the stopping criteria is satisfied. At that point the configuration will hopefully be in local potential energy minimum. More precisely, the configuration should approximate a critical point for the objective function (see below), which may or may not be a local minimum.

The minimization algorithm used is set by the min_style command. Other options are set by the min_modify command. Minimize commands can be interspersed with run commands to alternate between relaxation and dynamics. The minimizers bound the distance atoms move in one iteration, so that you can relax systems with highly overlapped atoms (large energies and forces) by pushing the atoms off of each other.

Alternate means of relaxing a system are to run dynamics with a small or limited timestep. Or dynamics can be run using fix viscous to impose a damping force that slowly drains all kinetic energy from the system. The pair_style soft potential can be used to un-overlap atoms while running dynamics.

The minimization styles cg, sd, and hftn involves an outer iteration loop which sets the search direction along which atom coordinates are changed. An inner iteration is then performed using a line search algorithm. The line search typically evaluates forces and energies several times to set new coordinates. Currently, a backtracking algorithm is used which may not be optimal in terms of the number of force evaluations performed, but appears to be more robust than previous line searches we've tried. The backtracking method is described in Nocedal and Wright's Numerical Optimization (Procedure 3.1 on p 41).

The minimization styles quickmin and fire perform damped dynamics using an Euler integration step. Thus they require a timestep be defined, typically the same value used for running dynamics with the system.

The objective function being minimized is the total potential energy of the system as a function of the N atom coordinates:
\[ E(r_1, r_2, \ldots, r_N) = \sum_{i,j} E_{\text{pair}}(r_i, r_j) + \sum_{ij} E_{\text{bond}}(r_i, r_j) + \sum_{ijk} E_{\text{angle}}(r_i, r_j, r_k) + \]
\[ \sum_{ijkl} E_{\text{dihedral}}(r_i, r_j, r_k, r_l) + \sum_{ijkl} E_{\text{improper}}(r_i, r_j, r_k, r_l) + \sum_{i} E_{\text{fix}} \]

where the first term is the sum of all non-bonded pairwise interactions including long-range Coulombic interactions, the 2nd thru 5th terms are bond, angle, dihedral, and improper interactions respectively, and the last term is energy due to fixes which can act as constraints or apply force to atoms, such as thru interaction with a wall. See the discussion below about how fix commands affect minimization.

The starting point for the minimization is the current configuration of the atoms.

The minimization procedure stops if any of several criteria are met:

- the change in energy between outer iterations is less than \( \text{etol} \)
- the 2-norm (length) of the global force vector is less than the \( \text{ftol} \)
- the line search fails because the step distance backtracks to 0.0
- the number of outer iterations or timesteps exceeds \( \text{maxiter} \)
- the number of total force evaluations exceeds \( \text{maxeval} \)

For the first criterion, the specified energy tolerance \( \text{etol} \) is unitless; it is met when the energy change between successive iterations divided by the energy magnitude is less than or equal to the tolerance. For example, a setting of 1.0e-4 for \( \text{etol} \) means an energy tolerance of one part in 10^4. For the damped dynamics minimizers this check is not performed for a few steps after velocities are reset to 0, otherwise the minimizer would prematurely converge.

For the second criterion, the specified force tolerance \( \text{ftol} \) is in force units, since it is the length of the global force vector for all atoms, e.g. a vector of size 3N for N atoms. Since many of the components will be near zero after minimization, you can think of \( \text{ftol} \) as an upper bound on the final force on any component of any atom. For example, a setting of 1.0e-4 for \( \text{ftol} \) means no x, y, or z component of force on any atom will be larger than 1.0e-4 (in force units) after minimization.

Either or both of the \( \text{etol} \) and \( \text{ftol} \) values can be set to 0.0, in which case some other criterion will terminate the minimization.

During a minimization, the outer iteration count is treated as a timestep. Output is triggered by this timestep, e.g. thermodynamic output or dump and restart files.

Using the \text{thermo\_style custom} command with the \text{fmax} or \text{fnorm} keywords can be useful for monitoring the progress of the minimization. Note that these outputs will be calculated only from forces on the atoms, and will not include any extra degrees of freedom, such as from the \text{fix box/relax} command.

Following minimization, a statistical summary is printed that lists which convergence criterion caused the minimizer to stop, as well as information about the energy, force, final line search, and and iteration counts. An example is as follows:

\text{Minimization stats:}
- Stopping criterion = max iterations
- Energy initial, next-to-last, final =
The 3 energy values are for before and after the minimization and on the next-to-last iteration. This is what the `etol` parameter checks.

The two-norm force values are the length of the global force vector before and after minimization. This is what the `ftol` parameter checks.

The max-component force values are the absolute value of the largest component (x,y,z) in the global force vector, i.e. the infinity-norm of the force vector.

The alpha parameter for the line-search, when multiplied by the max force component (on the last iteration), gives the max distance any atom moved during the last iteration. Alpha will be 0.0 if the line search could not reduce the energy. Even if alpha is non-zero, if the "max atom move" distance is tiny compared to typical atom coordinates, then it is possible the last iteration effectively caused no atom movement and thus the evaluated energy did not change and the minimizer terminated. Said another way, even with non-zero forces, it's possible the effect of those forces is to move atoms a distance less than machine precision, so that the energy cannot be further reduced.

The iterations and force evaluation values are what is checked by the `maxiter` and `maxeval` parameters.

IMPORTANT NOTE: There are several force fields in LAMMPS which have discontinuities or other approximations which may prevent you from performing an energy minimization to high tolerances. For example, you should use a pair style that goes to 0.0 at the cutoff distance when performing minimization (even if you later change it when running dynamics). If you do not do this, the total energy of the system will have discontinuities when the relative distance between any pair of atoms changes from cutoff+epsilon to cutoff-epsilon and the minimizer may behave poorly. Some of the manybody potentials use splines and other internal cutoffs that inherently have this problem. The long-range Coulombic styles (PPPM, Ewald) are approximate to within the user-specified tolerance, which means their energy and forces may not agree to a higher precision than the Kspace-specified tolerance. In all these cases, the minimizer may give up and stop before finding a minimum to the specified energy or force tolerance.

Note that a cutoff Lennard-Jones potential (and others) can be shifted so that its energy is 0.0 at the cutoff via the `pair_modify` command. See the doc pages for individual pair styles for details. Note that Coulombic potentials always have a cutoff, unless versions with a long-range component are used (e.g. pair_style lj/cut/coul/long). The CHARMM potentials go to 0.0 at the cutoff (e.g. pair_style lj/charmm/coul/charmm), as do the GROMACS potentials (e.g. pair_style lj/gromacs).

If a soft potential (pair_style soft) is used the Astop value is used for the prefactor (no time dependence).

The fix box/relax command can be used to apply an external pressure to the simulation box and allow it to shrink/expand during the minimization.

Only a few other fixes (typically those that apply force constraints) are invoked during minimization. See the doc pages for individual fix commands to see which ones are relevant.

IMPORTANT NOTE: Some fixes which are invoked during minimization have an associated potential energy. For that energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify energy option for that fix. The doc pages for individual fix commands specify if this
Restrictions:

Features that are not yet implemented are listed here, in case someone knows how they could be coded:

It is an error to use **fix shake** with minimization because it turns off bonds that should be included in the potential energy of the system. The effect of a fix shake can be approximated during a minimization by using stiff spring constants for the bonds and/or angles that would normally be constrained by the SHAKE algorithm.

**Fix rigid** is also not supported by minimization. It is not an error to have it defined, but the energy minimization will not keep the defined body(s) rigid during the minimization. Note that if bonds, angles, etc internal to a rigid body have been turned off (e.g. via **neigh_modify exclude**), they will not contribute to the potential energy which is probably not what is desired.

Pair potentials that produce torque on a particle (e.g. **granular potentials** or the **GayBerne potential** for ellipsoidal particles) are not relaxed by a minimization. More specifically, radial relaxations are induced, but no rotations are induced by a minimization, so such a system will not fully relax.

Related commands:

**min_modify, min_style, run_style**

Default: **none**
neb command

Syntax:

neb etol ftol N1 N2 Nevery filename

- etol = stopping tolerance for energy (energy units)
- ftol = stopping tolerance for force (force units)
- N1 = max # of iterations (timesteps) to run initial NEB
- N2 = max # of iterations (timesteps) to run barrier-climbing NEB
- Nevery = print replica energies and reaction coordinates every this many timesteps
- filename = file specifying final atom coordinates on other side of barrier

Examples:

neb 0.1 0.0 1000 500 50 coords.final
neb 0.0 0.001 1000 500 50 coords.final

Description:

Perform a nudged elastic band (NEB) calculation using multiple replicas of a system. Two or more replicas must be used, two of which are the end points of the transition path.

NEB is a method for finding both the atomic configurations and height of the energy barrier associated with a transition state, e.g. for an atom to perform a diffusive hop from one energy basin to another in a coordinated fashion with its neighbors. The implementation in LAMMPS follows the discussion in these 3 papers: (Henkelman1), (Henkelman2), and (Nakano).

Each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the -partition command-line switch; see Section_start 6 of the manual. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g you can run a 10-replica simulation on one or two processors. You will simply not get the performance speed-up you would see with one or more physical processors per replica. See this section of the manual for further discussion.

NOTE: The current NEB implementation in LAMMPS restricts you to having exactly one processor per replica.

When a NEB calculation is performed, it is assumed that each replica is running the same model, though LAMMPS does not check for this. I.e. the simulation domain, the number of atoms, the interaction potentials, and the starting configuration when the neb command is issued should be the same for every replica.

In a NEB calculation each atom in a replica is connected to the same atom in adjacent replicas by springs, which induce inter-replica forces. These forces are imposed by the fix neb command, which must be used in conjunction with the neb command. The group used to define the fix neb command specifies which atoms the inter-replica springs are applied to. These are the NEB atoms. Additional atoms can be present in your system, e.g. to provide a background force field or simply to hold fixed during the NEB procedure, but they will not be part of the barrier finding procedure.

The "starting configuration" for NEB should be a state with the NEB atoms (and all other atoms) having coordinates on one side of the energy barrier. These coordinates will be assigned to the first replica #1. The coordinates should be close to a local energy minimum. A perfect energy minimum is not required, since NEB
runs via damped dynamics which will tend to drive the configuration of replica #1 to a true energy minimum, but you will typically get better convergence if the initial state is already at a minimum. For example, for a system with a free surface, the surface should be fully relaxed before attempting a NEB calculation.

The final configuration is specified in the input filename, which is formatted as described below. Only coordinates for NEB atoms or a subset of them should be listed in the file; they represent the state of the system on the other side of the barrier, at or near an energy minimum. These coordinates will be assigned to the last replica #M. The final coordinates of atoms not listed in filename are set equal to their initial coordinates. Again, a perfect energy minimum is not required for the final configuration, since the atoms in replica #M will tend to move during the NEB procedure to the nearest energy minimum. Also note that a final coordinate does not need to be specified for a NEB atom if you expect it to only displace slightly during the NEB procedure. For example, only the final coordinate of the single atom diffusing into a vacancy need be specified if the surrounding atoms will only relax slightly in the final configuration.

The initial coordinates of all atoms (not just NEB atoms) in the intermediate replicas #2,#3,...,#M-1 are set to values linearly interpolated between the corresponding atoms in replicas #1 and #M.

A NEB calculation has two stages, each of which is a minimization procedure, performed via damped dynamics. To enable this, you must first define an appropriate min_style, such as quickmin or fire. The cg, sd, and hftn styles cannot be used, since they perform iterative line searches in their inner loop, which cannot be easily synchronized across multiple replicas.

The minimizer tolerances for energy and force are set by etol and ftol, the same as for the minimize command.

A non-zero etol means that the NEB calculation will terminate if the energy criterion is met by every replica. The energies being compared to etol do not include any contribution from the inter-replica forces, since these are non-conservative. A non-zero ftol means that the NEB calculation will terminate if the force criterion is met by every replica. The forces being compared to ftol include the inter-replica forces between an atom and its images in adjacent replicas.

The maximum number of iterations in each stage is set by N1 and N2. These are effectively timestep counts since each iteration of damped dynamics is like a single timestep in a dynamics run. During both stages, the potential energy of each replica and its normalized distance along the reaction path (reaction coordinate RD) will be printed to the screen and log file every Nevery timesteps. The RD is 0 and 1 for the first and last replica. For intermediate replicas, it is the cumulative distance (normalized by the total cumulative distance) between adjacent replicas, where "distance" is defined as the length of the 3N-vector of differences in atomic coordinates, where N is the number of NEB atoms involved in the transition. These outputs allow you to monitor NEB's progress in finding a good energy barrier. N1 and N2 must both be multiples of Nevery.

In the first stage of NEB, the set of replicas should converge toward the minimum energy path (MEP) of conformational states that transition over the barrier. The MEP for a barrier is defined as a sequence of 3N-dimensional states that cross the barrier at its saddle point, each of which has a potential energy gradient parallel to the MEP itself. The replica states will also be roughly equally spaced along the MEP due to the inter-replica spring force added by the fix neb command.

In the second stage of NEB, the replica with the highest energy is selected and the inter-replica forces on it are converted to a force that drives its atom coordinates to the top or saddle point of the barrier, via the barrier-climbing calculation described in (Henkelman2). As before, the other replicas rearrange themselves along the MEP so as to be roughly equally spaced.

When both stages are complete, if the NEB calculation was successful, one of the replicas should be an atomic configuration at the top or saddle point of the barrier, the potential energies for the set of replicas should represent
the energy profile of the barrier along the MEP, and the configurations of the replicas should be a sequence of configurations along the MEP.

A few other settings in your input script are required or advised to perform a NEB calculation.

An atom map must be defined which it is not by default for atom_style atomic problems. The atom_modify map command can be used to do this.

The "atom_modify sort 0 0.0" command should be used to turn off atom sorting.

NOTE: This sorting restriction will be removed in a future version of NEB in LAMMPS.

The minimizers in LAMMPS operate on all atoms in your system, even non-NEB atoms, as defined above. To prevent non-NEB atoms from moving during the minimization, you should use the fix setforce command to set the force on each of those atoms to 0.0. This is not required, and may not even be desired in some cases, but if those atoms move too far (e.g. because the initial state of your system was not well-minimized), it can cause problems for the NEB procedure.

The damped dynamics minimizers, such as quickmin and fire), adjust the position and velocity of the atoms via an Euler integration step. Thus you must define an appropriate timestep to use with NEB. Using the same timestep that would be used for a dynamics run of your system is advised.

The specified filename contains atom coordinates for the final configuration. Only atoms with coordinates different than the initial configuration need to be specified, i.e. those geometrically near the barrier.

The file can be ASCII text or a gzipped text file (detected by a .gz suffix). The file should contain one line per atom, formatted with the atom ID, followed by the final x,y,z coordinates:

<table>
<thead>
<tr>
<th>Atom ID</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>125</td>
<td>24.97311</td>
<td>1.69005</td>
<td>23.46956</td>
</tr>
<tr>
<td>126</td>
<td>1.94691</td>
<td>2.79640</td>
<td>1.92799</td>
</tr>
<tr>
<td>127</td>
<td>0.15906</td>
<td>3.46099</td>
<td>0.79121</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

The lines can be listed in any order.

Four kinds of output can be generated during a NEB calculation: energy barrier statistics, thermodynamic output by each replica, dump files, and restart files.

When running with multiple partitions (each of which is a replica in this case), the print-out to the screen and master log.lammps file contains a line of output, printed once every Nevery timesteps. It contains the timestep, the maximum force per replica, the maximum force per atom (in any replica), potential gradients in the initial, final, and climbing replicas, the forward and backward energy barriers, the total reaction coordinate (RDT), and the normalized reaction coordinate and potential energy of each replica.

The "maximum force per replica" is the two-norm of the 3N-length force vector for the atoms in each replica, maximized across replicas, which is what the ftol setting is checking against. In this case, N is all the atoms in each replica. The "maximum force per atom" is the maximum force component of any atom in any replica. The potential gradients are the two-norm of the 3N-length force vector solely due to the interaction potential i.e. without adding in inter-replica forces. Note that inter-replica forces are zero in the initial and final replicas, and only affect the direction in the climbing replica. For this reason, the "maximum force per replica" is often equal to the potential gradient in the climbing replica. In the first stage of NEB, there is no climbing replica, and so the potential gradient in the highest energy replica is reported, since this replica will become the climbing replica in the second stage of NEB.
The "reaction coordinate" (RD) for each replica is the two-norm of the 3N-length vector of distances between its atoms and the preceding replica's atoms, added to the RD of the preceding replica. The RD of the first replica RD1 = 0.0; the RD of the final replica RDN = RDT, the total reaction coordinate. The normalized RDs are divided by RDT, so that they form a monotonically increasing sequence from zero to one. When computing RD, N only includes the atoms being operated on by the fix neb command.

The forward (reverse) energy barrier is the potential energy of the highest replica minus the energy of the first (last) replica.

When running on multiple partitions, LAMMPS produces additional log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For a NEB calculation, these contain the thermodynamic output for each replica.

If dump commands in the input script define a filename that includes a universe or uloop style variable, then one dump file (per dump command) will be created for each replica. At the end of the NEB calculation, the final snapshot in each file will contain the sequence of snapshots that transition the system over the energy barrier. Earlier snapshots will show the convergence of the replicas to the MEP.

Likewise, restart filenames can be specified with a universe or uloop style variable, to generate restart files for each replica. These may be useful if the NEB calculation fails to converge properly to the MEP, and you wish to restart the calculation from an intermediate point with altered parameters.

There are 2 Python scripts provided in the tools/python directory, neb_combine.py and neb_final.py, which are useful in analyzing output from a NEB calculation. Assume a NEB simulation with M replicas, and the NEB atoms labelled with a specific atom type.

The neb_combine.py script extracts atom coords for the NEB atoms from all M dump files and creates a single dump file where each snapshot contains the NEB atoms from all the replicas and one copy of non-NEB atoms from the first replica (presumed to be identical in other replicas). This can be visualized/animated to see how the NEB atoms relax as the NEB calculation proceeds.

The neb_final.py script extracts the final snapshot from each of the M dump files to create a single dump file with M snapshots. This can be visualized to watch the system make its transition over the energy barrier.

To illustrate, here are images from the final snapshot produced by the neb_combine.py script run on the dump files produced by the two example input scripts in examples/neb. Click on them to see a larger image.

Restrictions:

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

Related commands:

prd, temper, fix langevin, fix viscous


neigh_modify command

Syntax:

neigh_modify keyword values ...

- one or more keyword/value pairs may be listed

keyword = delay or every or check or once or include or exclude or page or one or binsize
delay value = N
   N = delay building until this many steps since last build
every value = M
   M = build neighbor list every this many steps
check value = yes or no
   yes = only build if some atom has moved half the skin distance or more
   no = always build on 1st step that every and delay are satisfied
once
   yes = only build neighbor list once at start of run and never rebuild
   no = rebuild neighbor list according to other settings
include value = group-ID
   group-ID = only build pair neighbor lists for atoms in this group
exclude values:
   type M N
      M,N = exclude if one atom in pair is type M, other is type N
group group1-ID group2-ID
      group1-ID,group2-ID = exclude if one atom is in 1st group, other in 2nd
molecule group-ID
      groupname = exclude if both atoms are in the same molecule and in the same group
    none
    delete all exclude settings
page value = N
   N = number of pairs stored in a single neighbor page
one value = N
   N = max number of neighbors of one atom
binsize value = size
   size = bin size for neighbor list construction (distance units)

Examples:

neigh_modify every 2 delay 10 check yes page 100000
neigh_modify exclude type 2 3
neigh_modify exclude group frozen frozen check no
neigh_modify exclude group residue1 chain3
neigh_modify exclude molecule rigid

Description:

This command sets parameters that affect the building and use of pairwise neighbor lists.

The every, delay, check, and once options affect how often lists are built as a simulation runs. The delay setting means never build a new list until at least N steps after the previous build. The every setting means build the list every M steps (after the delay has passed). If the check setting is no, the list is built on the 1st step that satisfies the delay and every settings. If the check setting is yes, then the list is only built on a particular step if some atom has moved more than half the skin distance (specified in the neighbor command) since the last build. If the once setting is yes, then the neighbor list is only built once at the beginning of each run, and never rebuilt. This should only be done if you are certain atoms will not move far enough that the list should be rebuilt. E.g. running a
simulation of a cold crystal. Note that it is not that expensive to check if neighbor lists should be rebuilt.

When the rRESPA integrator is used (see the run_style command), the every and delay parameters refer to the longest (outermost) timestep.

The include option limits the building of pairwise neighbor lists to atoms in the specified group. This can be useful for models where a large portion of the simulation is particles that do not interact with other particles or with each other via pairwise interactions. The group specified with this option must also be specified via the atom_modify first command.

The exclude option turns off pairwise interactions between certain pairs of atoms, by not including them in the neighbor list. These are sample scenarios where this is useful:

- In crack simulations, pairwise interactions can be shut off between 2 slabs of atoms to effectively create a crack.
- When a large collection of atoms is treated as frozen, interactions between those atoms can be turned off to save needless computation. E.g. Using the fix setforce command to freeze a wall or portion of a bio-molecule.
- When one or more rigid bodies are specified, interactions within each body can be turned off to save needless computation. See the fix rigid command for more details.

The exclude type option turns off the pairwise interaction if one atom is of type M and the other of type N. M can equal N. The exclude group option turns off the interaction if one atom is in the first group and the other is the second. Group1-ID can equal group2-ID. The exclude molecule option turns off the interaction if both atoms are in the specified group and in the same molecule, as determined by their molecule ID.

Each of the exclude options can be specified multiple times. The exclude type option is the most efficient option to use; it requires only a single check, no matter how many times it has been specified. The other exclude options are more expensive if specified multiple times; they require one check for each time they have been specified.

Note that the exclude options only affect pairwise interactions; see the delete_bonds command for information on turning off bond interactions.

The page and one options affect how memory is allocated for the neighbor lists. For most simulations the default settings for these options are fine, but if a very large problem is being run or a very long cutoff is being used, these parameters can be tuned. The indices of neighboring atoms are stored in "pages", which are allocated one after another as they fill up. The size of each page is set by the page value. A new page is allocated when the next atom's neighbors could potentially overflow the list. This threshold is set by the one value which tells LAMMPS the maximum number of neighbor's one atom can have.

IMPORTANT NOTE: LAMMPS can crash without an error message if the number of neighbors for a single particle is larger than the page setting, which means it is much, much larger than the one setting. This is because LAMMPS doesn't error check these limits for every pairwise interaction (too costly), but only after all the particle's neighbors have been found. This problem usually means something is very wrong with the way you've setup your problem (particle spacing, cutoff length, neighbor skin distance, etc). If you really expect that many neighbors per particle, then boost the one and page settings accordingly.

The binsize option allows you to specify what size of bins will be used in neighbor list construction to sort and find neighboring atoms. By default, for neighbor style bin, LAMMPS uses bins that are 1/2 the size of the maximum pair cutoff. For neighbor style multi, the bins are 1/2 the size of the minimum pair cutoff. Typically these are good values values for minimizing the time for neighbor list construction. This setting overrides the default. If you make it too big, there is little overhead due to looping over bins, but more atoms are checked. If
you make it too small, the optimal number of atoms is checked, but bin overhead goes up. If you set the binsize to 0.0, LAMMPS will use the default binsize of 1/2 the cutoff.

**Restrictions:**

If the "delay" setting is non-zero, then it must be a multiple of the "every" setting.

The exclude molecule option can only be used with atom styles that define molecule IDs.

The value of the page setting must be at least 10x larger than the one setting. This insures neighbor pages are not mostly empty space.

**Related commands:**

neighbor, delete_bonds

**Default:**

The option defaults are delay = 10, every = 1, check = yes, once = no, include = all, exclude = none, page = 100000, one = 2000, and binsize = 0.0.
neighbor command

Syntax:

neighbor skin style

- skin = extra distance beyond force cutoff (distance units)
- style = bin or nsq or multi

Examples:

neighbor 0.3 bin
neighbor 2.0 nsq

Description:

This command sets parameters that affect the building of pairwise neighbor lists. All atom pairs within a neighbor cutoff distance equal to the their force cutoff plus the skin distance are stored in the list. Typically, the larger the skin distance, the less often neighbor lists need to be built, but more pairs must be checked for possible force interactions every timestep. The default value for skin depends on the choice of units for the simulation; see the default values below.

The skin distance is also used to determine how often atoms migrate to new processors if the check option of the neigh_modify command is set to yes. Atoms are migrated (communicated) to new processors on the same timestep that neighbor lists are re-built.

The style value selects what algorithm is used to build the list. The bin style creates the list by binning which is an operation that scales linearly with N/P, the number of atoms per processor where N = total number of atoms and P = number of processors. It is almost always faster than the nsq style which scales as (N/P)^2. For unsolvated small molecules in a non-periodic box, the nsq choice can sometimes be faster. Either style should give the same answers.

The multi style is a modified binning algorithm that is useful for systems with a wide range of cutoff distances, e.g. due to different size particles. For the bin style, the bin size is set to 1/2 of the largest cutoff distance between any pair of atom types and a single set of bins is defined to search over for all atom types. This can be inefficient if one pair of types has a very long cutoff, but other type pairs have a much shorter cutoff. For style multi the bin size is set to 1/2 of the shortest cutoff distance and multiple sets of bins are defined to search over for different atom types. This imposes some extra setup overhead, but the searches themselves may be much faster for the short-cutoff cases. See the communicate multi command for a communication option option that may also be beneficial for simulations of this kind.

The neigh_modify command has additional options that control how often neighbor lists are built and which pairs are stored in the list.

When a run is finished, counts of the number of neighbors stored in the pairwise list and the number of times neighbor lists were built are printed to the screen and log file. See this section for details.

Restrictions: none

Related commands:
neigh_modify, units, communicate

Default:

0.3 bin for units = lj, skin = 0.3 sigma
2.0 bin for units = real or metal, skin = 2.0 Angstroms
0.001 bin for units = si, skin = 0.001 meters = 1.0 mm
0.1 bin for units = cgs, skin = 0.1 cm = 1.0 mm
newton command

Syntax:

newton flag
newton flag1 flag2

- flag = on or off for both pairwise and bonded interactions
- flag1 = on or off for pairwise interactions
- flag2 = on or off for bonded interactions

Examples:

newton off
newton on off

Description:

This command turns Newton’s 3rd law on or off for pairwise and bonded interactions. For most problems, setting Newton's 3rd law to on means a modest savings in computation at the cost of two times more communication. Whether this is faster depends on problem size, force cutoff lengths, a machine's compute/communication ratio, and how many processors are being used.

Setting the pairwise newton flag to off means that if two interacting atoms are on different processors, both processors compute their interaction and the resulting force information is not communicated. Similarly, for bonded interactions, newton off means that if a bond, angle, dihedral, or improper interaction contains atoms on 2 or more processors, the interaction is computed by each processor.

LAMMPS should produce the same answers for any newton flag settings, except for round-off issues.

With run_style respa and only bonded interactions (bond, angle, etc) computed in the innermost timestep, it may be faster to turn newton off for bonded interactions, to avoid extra communication in the innermost loop.

Restrictions:

The newton bond setting cannot be changed after the simulation box is defined by a read_data or create_box command.

Related commands:

run_style respa

Default:

newton on
next command

Syntax:

next variables

• variables = one or more variable names

Examples:

next x
next a t x myTemp

Description:

This command is used with variables defined by the variable command. It assigns the next value to the variable from the list of values defined for that variable by the variable command. Thus when that variable is subsequently substituted for in an input script command, the new value is used.

See the variable command for info on how to define and use different kinds of variables in LAMMPS input scripts. If a variable name is a single lower-case character from "a" to "z", it can be used in an input script command as $a or $z. If it is multiple letters, it can be used as ${myTemp}.

If multiple variables are used as arguments to the next command, then all must be of the same variable style: index, loop, universe, or uloop. An exception is that universe- and uloop-style variables can be mixed in the same next command.

All the variables specified with the next command are incremented by one value from their respective list or values. String- or atom- or equal- or world-style variables cannot be used with the the next command, since they only store a single value.

When any of the variables in the next command has no more values, a flag is set that causes the input script to skip the next jump command encountered. This enables a loop containing a next command to exit. As explained in the variable command, the variable that has exhausted its values is also deleted. This allows it to be used and re-defined later in the input script.

When the next command is used with index- or loop-style variables, the next value is assigned to the variable for all processors. When the next command is used with universe- or uloop-style variables, the next value is assigned to whichever processor partition executes the command first. All processors in the partition are assigned the same value. Running LAMMPS on multiple partitions of processors via the "-partition" command-line switch is described in this section of the manual. Universe- and uloop-style variables are incremented using the files "tmp.lammps.variable" and "tmp.lammps.variable.lock" which you will see in your directory during such a LAMMPS run.

Here is an example of running a series of simulations using the next command with an index-style variable. If this input script is named in.polymer, 8 simulations would be run using data files from directories run1 thru run8.

variable d index run1 run2 run3 run4 run5 run6 run7 run8
shell cd $d
read_data data.polymer
run 10000
shell cd ..
If the variable "d" were of style *universe*, and the same in.polymer input script were run on 3 partitions of processors, then the first 3 simulations would begin, one on each set of processors. Whichever partition finished first, it would assign variable "d" the 4th value and run another simulation, and so forth until all 8 simulations were finished.

Jump and next commands can also be nested to enable multi-level loops. For example, this script will run 15 simulations in a double loop.

```
variable i loop 3
  variable j loop 5
  clear
  ...
  read_data data.polymer.$i$j
  print Running simulation $i.$j
  run 10000
  next j
  jump in.script
next i
jump in.script
```

Here is an example of a double loop which uses the *if* and *jump* commands to break out of the inner loop when a condition is met, then continues iterating thru the outer loop.

```
label       loopa
variable    a loop 5
label     loopb
variable  b loop 5
print   "A,B = $a,$b"
run    10000
if     $b > 2 then "jump in.script break"
next   b
jump    in.script loopb
label   break
variable b delete
next    a
jump   in.script loopa
```

**Restrictions:** none

**Related commands:**

*jump, include, shell, variable,*

**Default:** none
orient command

Syntax:

orient dim i j k

- dim = x or y or z
- i,j,k = orientation of lattice that is along box direction dim

Examples:

orient x 1 1 0
orient y -1 1 0
orient z 0 0 1

Description:

Specify the orientation of a cubic lattice along simulation box directions x or y or z. These 3 basis vectors are used when the create_atoms command generates a lattice of atoms.

The 3 basis vectors B1, B2, B3 must be mutually orthogonal and form a right-handed system such that B1 cross B2 is in the direction of B3.

The basis vectors should be specified in an irreducible form (smallest possible integers), though LAMMPS does not check for this.

Restrictions: none

Related commands:

origin, create_atoms

Default:

orient x 1 0 0
orient y 0 1 0
orient z 0 0 1
origin command

Syntax:

origin x y z

• x,y,z = origin of a lattice

Examples:

origin 0.0 0.5 0.5

Description:

Set the origin of the lattice defined by the lattice command. The lattice is used by the create_atoms command to create new atoms and by other commands that use a lattice spacing as a distance measure. This command offsets the origin of the lattice from the (0,0,0) coordinate of the simulation box by some fraction of a lattice spacing in each dimension.

The specified values are in lattice coordinates from 0.0 to 1.0, so that a value of 0.5 means the lattice is displaced 1/2 a cubic cell.

Restrictions: none

Related commands:

lattice, orient

Default:

origin 0 0 0
**package command**

**Syntax:**

```
package style args
```

- style = *gpu* or *cuda* or *omp*
- args = arguments specific to the style

**gpu args** = mode first last split keyword value ...  
  mode = force or force/neigh  
  first = ID of first GPU to be used on each node  
  last = ID of last GPU to be used on each node  
  split = fraction of particles assigned to the GPU  
  zero or more keyword/value pairs may be appended  
  keywords = `threads_per_atom`  
  `threads_per_atom` value = Nthreads  
  Nthreads = # of GPU threads used per atom  

**cuda args** = keyword value ...  
  one or more keyword/value pairs may be appended  
  keywords = `gpu/node` or `gpu/node/special` or `timing` or `test` or `override/bpa`  
  `gpu/node` value = N  
  N = number of GPUs to be used per node  
  `gpu/node/special` values = N gpu1 .. gpuN  
  N = number of GPUs to be used per node  
  gpu1 .. gpuN = N IDs of the GPUs to use  
  `timing` values = none  
  `test` values = id  
  id = atom-ID of a test particle  
  `override/bpa` values = flag  
  flag = 0 for TpA algorithm, 1 for BpA algorithm  

**omp args** = Nthreads mode  
  Nthreads = # of OpenMP threads to associate with each MPI process  
  mode = force or force/neigh (optional)

**Examples:**

```
package gpu force 0 0 1.0
package gpu force 0 0 0.75
package gpu force/neigh 0 0 1.0
package gpu force/neigh 0 1 -1.0
package cuda gpu/node/special 2 0 2
package cuda test 3948
package omp * force/neigh
package omp 4 force
```

**Description:**

This command invokes package-specific settings. Currently the following packages use it: GPU, USER-CUDA, and USER-OMP.

To use the accelerated GPU and USER-OMP styles, the use of the package command is required. However, as described in the "Defaults" section below, if you use the "-sf gpu" or "-sf omp" command-line options to enable use of these styles, then default package settings are enabled. In that case you only need to use the package command if you want to change the defaults.
To use the accelerate USER-CUDA styles, the package command is not required as defaults are assigned internally. You only need to use the package command if you want to change the defaults.

See Section_accelerate of the manual for more details about using these various packages for accelerating LAMMPS calculations.

The gpu style invokes options associated with the use of the GPU package.

The mode setting specifies where neighbor list calculations will be performed. If mode is force, neighbor list calculation is performed on the CPU. If mode is force/neigh, neighbor list calculation is performed on the GPU. GPU neighbor list calculation currently cannot be used with a triclinic box. GPU neighbor list calculation currently cannot be used with hybrid pair styles. GPU neighbor lists are not compatible with styles that are not GPU-enabled. When a non-GPU enabled style requires a neighbor list, it will also be built using CPU routines. In these cases, it will typically be more efficient to only use CPU neighbor list builds.

The first and last settings specify the GPUs that will be used for simulation. On each node, the GPU IDs in the inclusive range from first to last will be used.

The split setting can be used for load balancing force calculation work between CPU and GPU cores in GPU-enabled pair styles. If 0 < split < 1.0, a fixed fraction of particles is offloaded to the GPU while force calculation for the other particles occurs simultaneously on the CPU. If split = 1.0, all force calculations for GPU accelerated pair styles are performed on the GPU. In this case, hybrid, bond, angle, dihedral, improper, and long-range calculations can be performed on the CPU while the GPU is performing force calculations for the GPU-enabled pair style. If all CPU force computations complete before the GPU, LAMMPS will block until the GPU has finished before continuing the timestep.

As an example, if you have two GPUs per node and 8 CPU cores per node, and would like to run on 4 nodes (32 cores) with dynamic balancing of force calculation across CPU and GPU cores, you could specify

```plaintext
gpu force/neigh 0 1 -1
```

In this case, all CPU cores and GPU devices on the nodes would be utilized. Each GPU device would be shared by 4 CPU cores. The CPU cores would perform force calculations for some fraction of the particles at the same time the GPUs performed force calculation for the other particles.

The threads_per_atom keyword allows control of the number of GPU threads used per-atom to perform the short range force calculation. By default, the value will be chosen based on the pair style, however, the value can be set with this keyword to fine-tune performance. For large cutoffs or with a small number of particles per GPU, increasing the value can improve performance. The number of threads per atom must be a power of 2 and currently cannot be greater than 32.

The cuda style invokes options associated with the use of the USER-CUDA package.

The gpu/node keyword specifies the number N of GPUs to be used on each node. An MPI process with rank K will use the GPU (K mod N). This implies that processes should be assigned with successive ranks on each node, which is the default with most (or even all) MPI implementations. The default value for N is 2.

The gpu/node/special keyword also specifies the number (N) of GPUs to be used on each node, but allows more control over their specification. An MPI process with rank K will use the GPU gpuid with l = (K mod N) + 1. This implies that processes should be assigned with successive ranks on each node, which is the default with most (or even all) MPI implementations. For example if you have three GPUs on a machine, one of which is used for the X-Server (the GPU with the ID 1) while the others (with IDs 0 and 2) are used for computations you would
specify:

```
package cuda gpu/node/special 2 0 2
```

A main purpose of the `gpu/node/special` option is to allow two (or more) simulations to be run on one workstation. In that case one would set the first simulation to use GPU 0 and the second to use GPU 1. This is not necessary though, if the GPUs are in what is called `compute exclusive` mode. Using that setting, every process will get its own GPU automatically. This `compute exclusive` mode can be set as root using the `nvidia-smi` tool which is part of the CUDA installation.

Note that if the `gpu/node/special` keyword is not used, the USER-CUDA package sorts existing GPUs on each node according to their number of multiprocessors. This way, compute GPUs will be prioritized over X-Server GPUs.

Use of the `timing` keyword will output detailed timing information for various subroutines.

The `test` keyword will output info for the the specified atom at several points during each time step. This is mainly useful for debugging purposes. Note that the simulation will be severely slowed down if this option is used.

The `override/bpa` keyword can be used to specify which mode is used for pair-force evaluation. TpA = one thread per atom; BpA = one block per atom. If this keyword is not used, a short test at the begin of each run will determine which method is more effective (the result of this test is part of the LAMMPS output). Therefore it is usually not necessary to use this keyword.

The `omp` style invokes options associated with the use of the USER-OMP package.

The first argument allows to explicitly set the number of OpenMP threads to be allocated for each MPI process. For example, if your system has nodes with dual quad-core processors, it has a total of 8 cores per node. You could run MPI on 2 cores on each node (e.g. using options for the `mpirun` command), and set the `Nthreads` setting to 4. This would effectively use all 8 cores on each node. Since each MPI process would spawn 4 threads (one of which runs as part of the MPI process itself).

For performance reasons, you should not set `Nthreads` to more threads than there are physical cores (per MPI task), but LAMMPS cannot check for this.

An `Nthreads` value of `*` instructs LAMMPS to use whatever is the default for the given OpenMP environment. This is usually determined via the `OMP_NUM_THREADS` environment variable or the compiler runtime. Please note that in most cases the default for OpenMP capable compilers is to use one thread for each available CPU core when `OMP_NUM_THREADS` is not set, which can lead to extremely bad performance.

Which combination of threads and MPI tasks gives the best performance is difficult to predict and can depend on many components of your input. Not all features of LAMMPS support OpenMP and the parallel efficiency can be very different, too.

The `mode` setting specifies where neighbor list calculations will be multi-threaded as well. If `mode` is force, neighbor list calculation is performed in serial. If `mode` is force/neigh, a multi-threaded neighbor list build is used. Using the force/neigh setting is almost always faster and should produce identical neighbor lists at the expense of using some more memory (neighbor list pages are always allocated for all threads at the same time and each thread works on its own pages).

---

**Restrictions:**
This command cannot be used after the simulation box is defined by a `read_data` or `create_box` command.

The cuda style of this command can only be invoked if LAMMPS was built with the USER-CUDA package. See the Making LAMMPS section for more info.

The gpu style of this command can only be invoked if LAMMPS was built with the GPU package. See the Making LAMMPS section for more info.

The omp style of this command can only be invoked if LAMMPS was built with the USER-OMP package. See the Making LAMMPS section for more info.

Related commands:

suffix

Default:

If the `-sf gpu` command-line switch is used then it is as if the command "package gpu force/neigh 0 0 1" were invoked, to specify default settings for the GPU package. If the command-line switch is not used, then no defaults are set, and you must specify the appropriate package command in your input script.

The default settings for the USER CUDA package are "package cuda gpu 2". This is the case whether the `-sf cuda` command-line switch is used or not.

If the `-sf omp` command-line switch is used then it is as if the command "package omp *" were invoked, to specify default settings for the USER-OMP package. If the command-line switch is not used, then no defaults are set, and you must specify the appropriate package command in your input script.
pair_style adp command

pair_style adp/omp command

Syntax:

pair_style adp

Examples:

pair_style adp
pair_coeff * * Ta.adp Ta
pair_coeff * * ../potentials/AlCu.adp Al Al Cu

Description:

Style adp computes pairwise interactions for metals and metal alloys using the angular dependent potential (ADP) of (Mishin), which is a generalization of the embedded atom method (EAM) potential. The LAMMPS implementation is discussed in (Singh). The total energy $E_i$ of an atom I is given by

$$E_i = F_{\alpha} \left( \sum_{j \neq i} \rho_{\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij}) + \frac{1}{2} \sum_s \left( \mu^s_i \right)^2 + \frac{1}{2} \sum_{s,t} \left( \lambda^{st}_i \right)^2 - \frac{1}{6} \nu^2_i$$

$$\mu^s_i = \sum_{j \neq i} u_{\alpha\beta}(r_{ij}) r^s_{ij}$$

$$\lambda^{st}_i = \sum_{j \neq i} w_{\alpha\beta}(r_{ij}) r^s_{ij} r^t_{ij}$$

$$\nu_i = \sum_s \lambda^{ss}_i$$

where $F$ is the embedding energy which is a function of the atomic electron density rho, phi is a pair potential interaction, alpha and beta are the element types of atoms I and J, and $s$ and $t = 1, 2, 3$ and refer to the cartesian coordinates. The mu and lambda terms represent the dipole and quadruple distortions of the local atomic environment which extend the original EAM framework by introducing angular forces.

Note that unlike for other potentials, cutoffs for ADP potentials are not set in the pair_style or pair_coeff command; they are specified in the ADP potential files themselves. Likewise, the ADP potential files list atomic masses; thus you do not need to use the mass command to specify them.

The NIST WWW site distributes and documents ADP potentials:

http://www.ctcms.nist.gov/potentials

Note that these must be converted into the extended DYNAMO setfl format discussed below.
The NIST site is maintained by Chandler Becker (cbecker at nist.gov) who is a good resource for info on interatomic potentials and file formats.

Only a single pair_coeff command is used with the *adp* style which specifies an extended DYNAMO *setfl* file, which contains information for M elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of extended *setfl* elements to atom types

As an example, the potentials/AlCu.adp file, included in the potentials directory of the LAMMPS distribution, is an extended *setfl* file which has tabulated ADP values for w elements and their alloy interactions: Cu and Al. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Al, and the 4th to be Cu, you would use the following pair_coeff command:

```
pair_coeff * * AlCu.adp Al Al Al Cu
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Al arguments map LAMMPS atom types 1,2,3 to the Al element in the extended *setfl* file. The final Cu argument maps LAMMPS atom type 4 to the Al element in the extended *setfl* file. Note that there is no requirement that your simulation use all the elements specified by the extended *setfl* file.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when an *adp* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

*Adp* files in the *potentials* directory of the LAMMPS distribution have an ".adp" suffix. A DYNAMO *setfl* file extended for ADP is formatted as follows. Basically it is the standard *setfl* format with additional tabulated functions $u$ and $w$ added to the file after the tabulated pair potentials. See the pair_eam command for further details on the *setfl* format.

- lines 1,2,3 = comments (ignored)
- line 4: Nelements Element1 Element2 ... ElementN
- line 5: Nrho, drho, Nr, dr, cutoff

Following the 5 header lines are Nelements sections, one for each element, each with the following format:

- line 1 = atomic number, mass, lattice constant, lattice type (e.g. FCC)
- embedding function $F(\rho)$ (Nrho values)
- density function $\rho(r)$ (Nr values)

Following the Nelements sections, Nr values for each pair potential $\phi(r)$ array are listed for all i,j element pairs in the same format as other arrays. Since these interactions are symmetric ($i,j = j,i$) only phi arrays with $i \geq j$ are listed, in the following order: $i,j = (1,1), (2,1), (2,2), (3,1), (3,2), (3,3), (4,1), ...$, (Nelements, Nelements). The tabulated values for each phi function are listed as $r^3\phi$ (in units of eV-Angstroms), since they are for atom pairs, the same as for other EAM files.

After the $\phi(r)$ arrays, each of the $u(r)$ arrays are listed in the same order with the same assumptions of symmetry. Directly following the $u(r)$, the $w(r)$ arrays are listed. Note that $\phi(r)$ is the only array tabulated with a scaling by $r$. 

771
Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, no special mixing rules are needed, since the ADP potential files specify alloy interactions explicitly.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in tabulated potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default).

Related commands:

pair_coeff, pair_eam

Default: none


(Singh) Singh and Warner, Acta Mater, 58, 5797-5805 (2010),
pair_style airebo command

pair_style airebo/omp command

pair_style rebo command

pair_style rebo/omp command

Syntax:

pair_style style cutoff LJ_flag TORSION_flag

- style = airebo or rebo
- cutoff = LJ cutoff (sigma scale factor) (AIREBO only)
- LJ_flag = 0/1 to turn off/on the LJ term (AIREBO only, optional)
- TORSION_flag = 0/1 to turn off/on the torsion term (AIREBO only, optional)

Examples:

pair_style airebo 3.0
pair_style airebo 2.5 1 0
pair_coeff * * ../potentials/CH.airebo H C

pair_style rebo
pair_coeff * * ../potentials/CH.airebo H C

Description:

The airebo pair style computes the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) Potential of (Stuart) for a system of carbon and/or hydrogen atoms. Note that this is the initial formulation of AIREBO from 2000, not the later formulation. The rebo pair style computes the Reactive Empirical Bond Order (REBO) Potential of (Brenner). Note that this is the so-called 2nd generation REBO from 2002, not the original REBO from 1990. As discussed below, 2nd generation REBO is closely related to the initial AIREBO; it is just a subset of the potential energy terms.

The AIREBO potential consists of three terms:

\[
E = \frac{1}{2} \sum_{i} \sum_{j \neq i} \left[ E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k \neq i} \sum_{l \neq i,j} E_{kijl}^{TORSION} \right]
\]

By default, all three terms are included. For the airebo style, if the two optional flag arguments to the pair_style command are included, the LJ and torsional terms can be turned off. Note that both or neither of the flags must be included. If both of the LJ and torsional terms are turned off, it becomes the 2nd-generation REBO potential, with a small caveat on the spline fitting procedure mentioned below. This can be specified directly as pair_style rebo with no additional arguments.
The detailed formulas for this potential are given in (Stuart); here we provide only a brief description.

The \( E_{\text{REBO}} \) term has the same functional form as the hydrocarbon REBO potential developed in (Brenner). The coefficients for \( E_{\text{REBO}} \) in AIREBO are essentially the same as Brenner's potential, but a few fitted spline values are slightly different. For most cases the \( E_{\text{REBO}} \) term in AIREBO will produce the same energies, forces and statistical averages as the original REBO potential from which it was derived. The \( E_{\text{REBO}} \) term in the AIREBO potential gives the model its reactive capabilities and only describes short-ranged C-C, C-H and H-H interactions \((r < 2 \text{ Angstroms})\). These interactions have strong coordination-dependence through a bond order parameter, which adjusts the attraction between the I,J atoms based on the position of other nearby atoms and thus has 3- and 4-body dependence.

The \( E_{\text{LJ}} \) term adds longer-ranged interactions \((2 < r < \text{cutoff})\) using a form similar to the standard Lennard Jones potential. The \( E_{\text{LJ}} \) term in AIREBO contains a series of switching functions so that the short-ranged LJ repulsion \((1/r^{12})\) does not interfere with the energetics captured by the \( E_{\text{REBO}} \) term. The extent of the \( E_{\text{LJ}} \) interactions is determined by the cutoff argument to the pair_style command which is a scale factor. For each type pair (C-C, C-H, H-H) the cutoff is obtained by multiplying the scale factor by the sigma value defined in the potential file for that type pair. In the standard AIREBO potential, \( \sigma_{\text{CC}} = 3.4 \) Angstroms, so with a scale factor of 3.0 (the argument in pair_style), the resulting \( E_{\text{LJ}} \) cutoff would be 10.2 Angstroms.

The \( E_{\text{TORSION}} \) term is an explicit 4-body potential that describes various dihedral angle preferences in hydrocarbon configurations.

Only a single pair_coeff command is used with the airebo or rebo style which specifies an AIREBO potential file with parameters for C and H. Note that the rebo style in LAMMPS uses the same AIREBO-formatted potential file. These are mapped to LAMMPS atom types by specifying \( N \) additional arguments after the filename in the pair_coeff command, where \( N \) is the number of LAMMPS atom types:

\[
\begin{align*}
\text{• filename} \\
\text{• } N \text{ element names } &= \text{ mapping of AIREBO elements to atom types}
\end{align*}
\]

As an example, if your LAMMPS simulation has 4 atom types and you want the 1st 3 to be C, and the 4th to be H, you would use the following pair_coeff command:

```
pair_coeff * * CH.airebo C C C H
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three C arguments map LAMMPS atom types 1,2,3 to the C element in the AIREBO file. The final H argument maps LAMMPS atom type 4 to the H element in the SW file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a airebo potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The parameters/coefficients for the AIREBO potentials are listed in the CH.airebo file to agree with the original (Stuart) paper. Thus the parameters are specific to this potential and the way it was fit, so modifying the file should be done cautiously.

Styles with a \texttt{cuda}, \texttt{gpu}, \texttt{omp}, or \texttt{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.
You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support the pair_modify mix, shift, table, and tail options.

These pair styles do not write their information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

These pair styles can only be used via the pair keyword of the run_style respa command. They do not support the inner, middle, outer keywords.

Restrictions:

These pair styles are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

These pair potentials require the newton setting to be "on" for pair interactions.

The CH.airebo potential file provided with LAMMPS (see the potentials directory) is parameterized for metal units. You can use the AIREBO or REBO potential with any LAMMPS units, but you would need to create your own AIREBO potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none


**pair_style awpmd/cut command**

**Syntax:**

```
pair_style awpmd/cut Rc keyword value ...
```

- **Rc** = global cutoff, -1 means cutoff of half the shortest box length
- zero or more keyword/value pairs may be appended
- **keyword** = *hartree* or *dproduct* or *uhf* or *free* or *pbc* or *fix* or *harm* or *ermyscale* or *flex_press*

```latex
\begin{align*}
\text{hartree} & \text{ value } = \text{none} \\
\text{dproduct} & \text{ value } = \text{none} \\
\text{uhf} & \text{ value } = \text{none} \\
\text{free} & \text{ value } = \text{none} \\
\text{pbc} & \text{ value } = \text{Plen} \\
\quad \text{Plen} & \text{ = periodic width of electron } = \text{-1 or positive value } (\text{distance units}) \\
\text{fix} & \text{ value } = \text{Flen} \\
\quad \text{Flen} & \text{ = fixed width of electron } = \text{-1 or positive value } (\text{distance units}) \\
\text{harm} & \text{ value } = \text{width} \\
\quad \text{width} & \text{ = harmonic width constraint} \\
\text{ermyscale} & \text{ value } = \text{factor} \\
\quad \text{factor} & \text{ = scaling between electron mass and width variable mass} \\
\text{flex_press} & \text{ value } = \text{none}
\end{align*}
```

**Examples:**

- `pair_style awpmd/cut -1`
- `pair_style awpmd/cut 40.0 uhf free`
- `pair_coeff * *`
- `pair_coeff 2 2 20.0`

**Description:**

This pair style contains an implementation of the Antisymmetrized Wave Packet Molecular Dynamics (AWPMD) method. Need citation here. Need basic formulas here. Could be links to other documents.

- **Rc** is the cutoff.

The `pair_style` command allows for several optional keywords to be specified.

The `hartree`, `dproduct`, and `uhf` keywords specify the form of the initial trial wave function for the system. If the `hartree` keyword is used, then a Hartree multielectron trial wave function is used. If the `dproduct` keyword is used, then a trial function which is a product of two determinants for each spin type is used. If the `uhf` keyword is used, then an unrestricted Hartree-Fock trial wave function is used.

The `free`, `pbc`, and `fix` keywords specify a width constraint on the electron wavepackets. If the `free` keyword is specified, then there is no constraint. If the `pbc` keyword is used and `Plen` is specified as -1, then the maximum width is half the shortest box length. If `Plen` is a positive value, then the value is the maximum width. If the `fix` keyword is used and `Flen` is specified as -1, then electrons have a constant width that is read from the data file. If `Flen` is a positive value, then the constant width for all electrons is set to `Flen`.

The `harm` keyword allow oscillations in the width of the electron wavepackets. More details are needed.
The `ermscale` keyword specifies a unitless scaling factor between the electron masses and the width variable mass. More details needed.

If the `flex_press` keyword is used, then a contribution from the electrons is added to the total virial and pressure of the system.

This potential is designed to be used with `atom_style wavepacket` definitions, in order to handle the description of systems with interacting nuclei and explicit electrons.

The following coefficients must be defined for each pair of atoms types via the `pair_coeff` command as in the examples above, or in the data file or restart files read by the `read_data` or `read_restart` commands, or by mixing as described below:

- `cutoff` (distance units)

For `awpmd/cut`, the cutoff coefficient is optional. If it is not used (as in some of the examples above), the default global value specified in the pair_style command is used.

---

**Mixing, shift, table, tail correction, restart, rRESPA info:**

The `pair_modify` mix, shift, table, and tail options are not relevant for this pair style.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner`, `middle`, `outer` keywords.

**Restrictions:** none

**Related commands:**

`pair_coeff`

**Default:**

These are the defaults for the pair_style keywords: `hartree` for the initial wavefunction, `free` for the wavepacket width.
pair_style beck command

pair_style beck/omp command

Syntax:

```
pair_style beck Rc
```

- Rc = cutoff for interactions (distance units)

Examples:

```
pair_style beck 8.0
pair_coeff * * 399.671876712 0.0000867636112694 0.675 4.390 0.0003746
pair_coeff 1 1 399.671876712 0.0000867636112694 0.675 4.390 0.0003746 6.0
```

Description:

Style `beck` computes interactions based on the potential by (Beck), originally designed for simulation of Helium. It includes truncation at a cutoff distance Rc.

\[
E(r) = A \exp \left[ -\alpha r - \beta r^6 \right] - \frac{B}{(r^2 + a^2)^3} \left( 1 + \frac{2.709 + 3a^2}{r^2 + a^2} \right) \quad r < R_c
\]

The following coefficients must be defined for each pair of atoms types via the `pair_coeff` command as in the examples above, or in the data file or restart files read by the `read_data` or `read_restart` commands.

- A (energy units)
- B (energy-distance^6 units)
- a (distance units)
- alpha (1/distance units)
- beta (1/distance^6 units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff Rc is used.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.
See Section _accelerate_ of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I != J, coeffiecients must be specified. No default mixture rules are used.

This pair style does not support the `pair_modify` shift option for the energy of the pair interaction.

The `pair_modify` table option is not relevant for this pair style.

This pair style does not support the `pair_modify` tail option for adding long-range tail corrections.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner, middle, outer` keywords.

**Restrictions:** none

**Related commands:**

`pair_coeff`

**Default:** none

(Beck) Beck, Molecular Physics, 14, 311 (1968).
pair_style bop command

Syntax:

pair_style bop keyword ...

- zero or more keywords may be appended
- keyword = table or save or sigmaoff

  table = BOP potential file has tabulated form
  save = pre-compute and save some values
  sigmaoff = assume a_sigma = 0

Examples:

pair_style bop
pair_coeff * * ../potentials/CdTe_bop Cd Te
pair_style bop table save
pair_coeff * * ../potentials/CdTe_bop.table Cd Te Te
communicate single cutoff 14.70

Description:

The bop pair style computes Bond-Order Potentials (BOP) based on quantum mechanical theory incorporating both sigma and pi bondings. By analytically deriving the BOP from quantum mechanical theory its transferability to different phases can approach that of quantum mechanical methods. This particular BOP is extremely effective at modeling III-V and II-VI compounds such as GaAs and CdTe. This potential is similar to the original BOP developed by Pettifor (Pettifor_1, Pettifor_2, Pettifor_3) and later updated by Murdick, Zhou, and Ward (Murdick, Ward).

The BOP potential consists of three terms:

\[
E = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{i} \phi_{ij}(r_{ij}) - \sum_{i=1}^{N} \sum_{j=1}^{i} \beta_{\sigma,ij}(r_{ij}) \cdot \Theta_{\sigma,ij} - \sum_{i=1}^{N} \sum_{j=1}^{i} \beta_{\pi,ij}(r_{ij}) \cdot \Theta_{\pi,ij} + U_{prom}
\]

where \( \phi_{ij}(r_{ij}) \) is a short-range two-body function representing the repulsion between a pair of ion cores, \( \beta_{(sigma,ij)}(r_{ij}) \) and \( \beta_{(phi,ij)(r_{ij})} \) are respectively sigma and pi bond integrals, \( \Theta_{(sigma,ij)} \) and \( \Theta_{(pi,ij)} \) are sigma and pi bond-orders, and \( U_{prom} \) is the promotion energy for sp-valent systems.

The detailed formulas for this potential are given in Ward (Ward); here we provide only a brief description.

The repulsive energy \( \phi_{ij}(r_{ij}) \) and the bond integrals \( \beta_{(sigma,ij)}(r_{ij}) \) and \( \beta_{(phi,ij)}(r_{ij}) \) are functions of the interatomic distance \( r_{ij} \) between atom i and j. Each of these potentials has a smooth cutoff at a radius of \( r_{(cut,ij)} \). These smooth cutoffs ensure stable behavior at situations with high sampling near the cutoff such as melts and surfaces.

The bond-orders can be viewed as environment-dependent local variables that are ij bond specific. The maximum value of the sigma bond-order (\( \Theta_{sigma} \)) is 1, while that of the pi bond-order (\( \Theta_{pi} \)) is 2, attributing to a maximum value of the total bond-order (\( \Theta_{sigma} + \Theta_{pi} \)) of 3. The sigma and pi bond-orders
reflect the ubiquitous single-, double-, and triple- bond behavior of chemistry. Their analytical expressions can be
derived from tight- binding theory by recursively expanding an inter-site Green's function as a continued fraction.
To accurately represent the bonding with a computationally efficient potential formulation suitable for MD
simulations, the derived BOP only takes (and retains) the first two levels of the recursive representations for both
the sigma and the pi bond-orders. Bond-order terms can be understood in terms of molecular orbital hopping
paths based upon the Cyrot-Lackmann theorem (Pettifor_1). The sigma bond-order with a half-full valence band
filling. This pi bond-order expression also contains also contains a three-member ring term that allows
implementation of an asymmetric density of states, which helps to either stabilize or destabilize close-packed
structures. The pi bond-order includes hopping paths of length 4. This enables the incorporation of dihedral angles
effects.

The cutoffs for the various interactions are defined in the BOP potential file.

IMPORTANT NOTE: You must use the communicate cutoff command to insure ghost atoms are acquired at a
distance 3x further than the largest BOP cutoff (for a particular pair of elements). E.g. if the BOP cutoff is 4.9
Angstroms, then the ghost atom communication needs to be 14.7 Angstroms or greater as in the example above.
This is because the BOP formulation uses neighbors of neighbors of neighbors to enumerate all the required
many-body interactions. LAMMPS will generate an error if you do not use an appropriate setting for the
communicate cutoff command.

Several options can be specified as keywords with the pair_style command.

The table keyword tells LAMMPS what format the BOP potential file is in. The default is a non-tabulated form. If
the table keyword is used, the file is in a tabulated form containing pre-tabulated pair functions for phi_ij(r_ij),
beta_(sigma,ij)(r_ij), and beta_(pi,ij)(r_ij). This allows you to use your own functional form for various
interactions.

The save keyword gives you the option to calculate and store in advance a set of distances, angles, and derivatives
of angles. The default is to not do this, but to calculate the various quantities on-the-fly each time they are needed.
The former may be faster, but takes more memory. The latter requires less memory, but may be slower. It is best
to test this option to see if it makes a difference on your machine for the specific problem you are modeling.

The sigmaoff keyword optimizes the BOP equations for the case of a_sigma = 0. For some published BOP
potentials, a_sigma = 0 and several terms in the BOP equationas drop out. If this is the case, specifying sigmaoff
will typically speed up the BOP pair style.

Only a single pair_coeff command is used with the bop style which specifies a BOP potential file, with
parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional
arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of BOP elements to atom types

As an example, imagine the CdTe.bop file has BOP values for Cd and Te. If your LAMMPS simulation has 4
atoms types and you want the 1st 3 to be Cd, and the 4th to be Te, you would use the following pair_coeff
command:

pair_coeff * * CdTe Cd Cd Cd Te

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Cd arguments map
LAMMPS atom types 1,2,3 to the Cd element in the BOP file. The final Te argument maps LAMMPS atom type
4 to the Te element in the BOP file. If a mapping value is specified as NULL, the mapping is not performed. This
can be used when a *bop* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

BOP files in the *potentials* directory of the LAMMPS distribution have a ".bop" or ".bop.table" suffix, depending on whether they are of the non-tabulated or tabulated form, as described above.

The parameters/coefficients format for the both kinds of BOP files are given below with variables matching the formulation of Ward (Ward). Each header line containing a ".:" is preceded by a blank line.

- Line 1: elements: (header)
- Line 2: #elements $N$

The first two lines are followed by $N$ lines containing the atomic number and mass of each element.

---

**Non-tabulated potential file format:**

Following the definition of the elements is the block of global variables for spline and quadratic fits of $\text{THETA}_{(S,ij)}$ and its components $\text{THETA}_0$, $\text{THETA}_1$, and $S$.

- Line 1: global: (header)
- Line 2: delta_1-delta_7 (if all are not used in the particular formulation, set unused values to 0.0)
- Line 3: ncutoff, r_big, r_small (r_big and r_small are parameters for pairwise paramters gamma typically set to 0.99 and 0.01, respectively)
- Line 4: which, alpha, nfunc (these are options for the spline which=1.0 (means using a smooth function); which=2.0 (spline), alpha is a parameter in the spline, nfunc is the type of GSP function ($f_{ij}$) (nfunc=1 is the published equation from Ward (Ward); nfunc=2 $f_{ij}(r_{ij})=\exp(n_{ij}r_{ij})$; nfunc=3 $f_{ij}(r_{ij})=1/(r_{ij})^{n_{ij}}$).
- Line 5: alpha_1, beta_1, gamma_1 ($\alpha_1=\text{first coefficient for THETA}_0$; $\beta_1=\text{first exponent for THETA}_0$; $\gamma_1=\text{second exponent for THETA}_0$)
- Line 6: alpha_2, beta_2 ($\alpha_2=\text{second coefficient for S}$; $\beta_2=\text{first exponent for S}$)
- Line 7: alpha_3, beta_3 ($\alpha_3=\text{first coefficient for THETA}_1$; $\beta_3=\text{second coefficient for THETA}_1$)

The next block contains constants for the environment depend promotional energy for sp-valent systems, each of which are species dependent. Refer to Pettifor (Pettifor_3) for constant definitions. As well as one species dependent parameter $p_{\pi i}$.

- Line 1: ptrs: (header)

Following the ptrs header there are $N$ lines for $e_{1-e_N}$ containing $(A_{ij})^{(\mu*\nu)}$, delta$^\mu$, $p_{\pi i}$

- Line 2: $(A_{ij})^{(\mu*\nu)}$, delta$^\mu$, $p_{\pi i}$ (for $e_{1}$)
- Line 3: $(A_{ij})^{(\mu*\nu)}$, delta$^\mu$, $p_{\pi i}$ (for $e_{2}$ and continues to $e_{N}$)

The next block contains constants for the pair interactions.

- Line 1: pairs: (header)

Following the header the block contains a series of constants for the number of pair interaction types, the block will be broken up into parameters for $e_{i-e_j}$ with $i=0->N$, $j=i->N$. Each single interaction section for this block will contain (see Ward for parameter definitions):
• Line 2: \( r_0, r_c, r_1, r_{\text{cut}} \) (for \( e_1-e_2 \) interactions)
• Line 3: \( m, n, n_c \)
• Line 4: \( \phi_0, \beta_{(\sigma,0)}, \beta_{(\pi,0)} \)
• Line 5: \( a_{\sigma}, c_{\sigma}, \delta_{\sigma} \) (From complete formulation of 1/2 full valance shell for this particular formulation \( \delta_{\sigma}=0 \))
• Line 6: \( a_{\pi}, c_{\pi}, \delta_{\pi} \)
• Line 7: \( f_{\sigma}, k_{\sigma}, \delta_3 \) (This \( \delta_3 \) is similar to that of the previous section but is interaction type dependent)
• Line 8: \( r_0, r_c, r_1, r_{\text{cut}} \) (for \( e_1-e_2 \) interactions and repeats as above)

The next block contains tris.

• Line 1: tris: (header)

Following the header there is a line for each three body interaction types as \( e_j-e_i-e_k \) with \( i->N, j->N, k=j->N \)

• Line 2: \( g_{\sigma 0}, g_{\sigma 1}, g_{\sigma 2} \) (these are coefficients for \( g_{(\sigma,ijk)}(\theta_{ijk}) \) for \( e_1-e_1-e_1 \) interaction. \textit{Ward} contains the full expressions for the constants as functions of \( b_{(\sigma,ijk)}, p_{(\sigma,ijk)}, u_{(\sigma,ijk)} \)
• Line 3: \( g_{\sigma 0}, g_{\sigma 1}, g_{\sigma 2} \) (for \( e_1-e_1-e_2 \))

This would be the end of the potential parameter file without pre-tabulated data.

---

**Tabulated potential file format:**

The parameters/coefficients format for the BOP potentials input file containing pre-tabulated functions of is given below with variables matching the formulation of \textit{Ward}.

• Line 1: \# elements N

The first two lines are followed by N lines containing the atomic number and mass of each element THETA_0 and THETA_1 (see \textit{Ward}).

Following the definition of the elements several global variables for the tabulated functions are given.

• Line 1: \( n_r, n_{\text{BoT}} \) (\( n_r \) is the number of divisions the radius is broken into for function tables and MUST be a factor of 5; \( n_{\text{BoT}} \) is the number of divisions for the tabulated values of THETA_(S,ij)
• Line 2: \( \delta_1-\delta_7 \) (if all are not used in the particular formulation, set unused values to 0.0)

Following this N lines for \( e_1-e_N \) containing \( p_{\pi} \).

• Line 3: \( p_{\pi} \) (for \( e_1 \))
• Line 4: \( p_{\pi} \) (for \( e_2 \) and continues to \( e_N \))

The next section contains several pair constants for the number of interaction types \( e_i-e_j \), with \( i=1->N, j=i->N \)

• Line 1: \( r_{\text{cut}} \) (for \( e_1-e_1 \) interactions)
• Line 2: \( c_{\sigma}, a_{\sigma}, c_{\pi}, a_{\pi} \)
• Line 3: \( \delta_{\sigma}, \delta_{\pi} \)
• Line 4: \( f_{\sigma}, k_{\sigma}, \delta_3 \) (This \( \delta_3 \) is similar to that of the previous section but is interaction type dependent)
The next section contains a line for each three body interaction type $e_{j}-e_{i}-e_{k}$ with $i=0\rightarrow N$, $j=0\rightarrow N$, $k=j\rightarrow N$

- Line 1: $g_{(\sigma_{0})}$, $g_{(\sigma_{1})}$, $g_{(\sigma_{2})}$ (These are coefficients for $g_{(\sigma,jik)}(\Theta_{ijk})$ for $e_{1}-e_{1}-e_{1}$ interaction. Ward contains the full expressions for the constants as functions of $b_{(\sigma,jik)}$, $p_{(\sigma,jik)}$, $u_{(\sigma,jik)}$)
- Line 2: $g_{(\sigma_{0})}$, $g_{(\sigma_{1})}$, $g_{(\sigma_{2})}$ (for $e_{1}-e_{1}-e_{2}$)

The next section contains a block for each interaction type for the $\phi_{ij}(r_{ij})$. Each block has $nr$ entries with 5 entries per line.

- Line 1: $\phi_{(r1)}$, $\phi_{(r2)}$, $\phi_{(r3)}$, $\phi_{(r4)}$, $\phi_{(r5)}$ (for the $e_{1}-e_{1}$ interaction type)
- Line 2: $\phi_{(r6)}$, $\phi_{(r7)}$, $\phi_{(r8)}$, $\phi_{(r9)}$, $\phi_{(r10)}$ (this continues until $nr$)
- ...
- Line $nr/5+1$: $\phi_{(r1)}$, $\phi_{(r2)}$, $\phi_{(r3)}$, $\phi_{(r4)}$, $\phi_{(r5)}$, (for the $e_{1}-e_{1}$ interaction type)

The next section contains a block for each interaction type for the $\beta_{(\sigma,ij)}(r_{ij})$. Each block has $nr$ entries with 5 entries per line.

- Line 1: $\beta_{\sigma}(r1)$, $\beta_{\sigma}(r2)$, $\beta_{\sigma}(r3)$, $\beta_{\sigma}(r4)$, $\beta_{\sigma}(r5)$ (for the $e_{1}-e_{1}$ interaction type)
- Line 2: $\beta_{\sigma}(r6)$, $\beta_{\sigma}(r7)$, $\beta_{\sigma}(r8)$, $\beta_{\sigma}(r9)$, $\beta_{\sigma}(r10)$ (this continues until $nr$)
- ...
- Line $nr/5+1$: $\beta_{\sigma}(r1)$, $\beta_{\sigma}(r2)$, $\beta_{\sigma}(r3)$, $\beta_{\sigma}(r4)$, $\beta_{\sigma}(r5)$ (for the $e_{1}-e_{2}$ interaction type)

The next section contains a block for each interaction type for $\beta_{(\pi,ij)}(r_{ij})$. Each block has $nr$ entries with 5 entries per line.

- Line 1: $\beta_{\pi}(r1)$, $\beta_{\pi}(r2)$, $\beta_{\pi}(r3)$, $\beta_{\pi}(r4)$, $\beta_{\pi}(r5)$ (for the $e_{1}-e_{1}$ interaction type)
- Line 2: $\beta_{\pi}(r6)$, $\beta_{\pi}(r7)$, $\beta_{\pi}(r8)$, $\beta_{\pi}(r9)$, $\beta_{\pi}(r10)$ (this continues until $nr$)
- ...
- Line $nr/5+1$: $\beta_{\pi}(r1)$, $\beta_{\pi}(r2)$, $\beta_{\pi}(r3)$, $\beta_{\pi}(r4)$, $\beta_{\pi}(r5)$ (for the $e_{1}-e_{2}$ interaction type)

The next section contains a block for each interaction type for $\Theta_{(S,ij)}(\Theta_{(\sigma,ij)}^{1/2}, f_{(\sigma,ij)})$. Each block has $nBOt$ entries with 5 entries per line.

- Line 1: $\Theta_{(S,ij)}(r1)$, $\Theta_{(S,ij)}(r2)$, $\Theta_{(S,ij)}(r3)$, $\Theta_{(S,ij)}(r4)$, $\Theta_{(S,ij)}(r5)$ (for the $e_{1}-e_{2}$ interaction type)
- Line 2: $\Theta_{(S,ij)}(r6)$, $\Theta_{(S,ij)}(r7)$, $\Theta_{(S,ij)}(r8)$, $\Theta_{(S,ij)}(r9)$, $\Theta_{(S,ij)}(r10)$ (this continues until $nBOt$)
- ...
- Line $nBOt/5+1$: $\Theta_{(S,ij)}(r1)$, $\Theta_{(S,ij)}(r2)$, $\Theta_{(S,ij)}(r3)$, $\Theta_{(S,ij)}(r4)$, $\Theta_{(S,ij)}(r5)$ (for the $e_{1}-e_{2}$ interaction type)

The next section contains a block of $N$ lines for $e_{1}-e_{N}$

- Line 1: $\delta^{\mu}$ (for $e_{1}$)
- Line 2: $\delta^{\mu}$ (for $e_{2}$ and repeats to $e_{N}$)

The last section contains more constants for $e_{i}-e_{j}$ interactions with $i=0\rightarrow N$, $j=i\rightarrow N$
Mixing, shift, table tail correction, restart:

This pair style does not support the \texttt{pair\_modify} mix, shift, table, and tail options.

This pair style does not write its information to \texttt{binary restart files}, since it is stored in potential files. Thus, you need to re-specify the \texttt{pair\_style} and \texttt{pair\_coeff} commands in an input script that reads a restart file.

This pair style can only be used via the \texttt{pair} keyword of the \texttt{run\_style respa} command. It does not support the \texttt{inner}, \texttt{middle}, \texttt{outer} keywords.

Restrictions:

These pair styles are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package (which it is by default). See the \texttt{Making LAMMPS} section for more info.

These pair potentials require the \texttt{newtion} setting to be "on" for pair interactions.

The CdTe.bop and GaAs.bop potential files provided with LAMMPS (see the potentials directory) are parameterized for metal \texttt{units}. You can use the BOP potential with any LAMMPS units, but you would need to create your own BOP potential file with coefficients listed in the appropriate units if your simulation does not use "metal" units.

Related commands:

- \texttt{pair\_coeff}

Default:

- \texttt{non-tabulated potential file, a\_0 is non-zero.}


pair_style born command

pair_style born/omp command

pair_style born/gpu command

pair_style born/coul/long command

pair_style born/coul/long/cuda command

pair_style born/coul/long/gpu command

pair_style born/coul/long/omp command

pair_style born/coul/wolf command

pair_style born/coul/wolf/gpu command

pair_style born/coul/wolf/omp command

Syntax:

pair_style style args

- style = born or born/coul/long or born/coul/wolf
- args = list of arguments for a particular style

born args = cutoff
    cutoff = global cutoff for non-Coulombic interactions (distance units)

born/coul/long args = cutoff (cutoff2)
    cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)

born/coul/wolf args = alpha cutoff (cutoff2)
    alpha = damping parameter (inverse distance units)
    cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)

Examples:

pair_style born 10.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/long 10.0
pair_style born/coul/long 10.0 8.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/wolf 0.25 10.0
pair_style born/coul/wolf 0.25 10.0 9.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
**Description:**

The *born* style computes the Born-Mayer-Huggins or Tosi/Fumi potential described in *(Fumi and Tosi)*, given by

\[
E = A \exp \left( \frac{\sigma - r}{\rho} \right) - \frac{C}{r^6} + \frac{D}{r^8} \quad r < r_c
\]

where \( \sigma \) is an interaction-dependent length parameter, \( \rho \) is an ionic-pair dependent length parameter, and \( r_c \) is the cutoff.

The *born/coul/long* style adds a Coulombic term as described for the *coul/long* pair style. An additional damping factor is applied to the Coulombic term so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

If one cutoff is specified for the *born/coul/long* style, it is used for both the A,C,D and Coulombic terms. If two cutoffs are specified, the first is used as the cutoff for the A,C,D terms, and the second is the cutoff for the Coulombic term.

The *born/coul/wolf* style adds a Coulombic term as described for the Wolf potential in the *coul/wolf* pair style.

If one cutoff is specified for the *born/coulk/long* style, it is used for both the A,C,D and Coulombic terms. If two cutoffs are specified, the first is used as the cutoff for the A,C,D terms, and the second is the cutoff for the Coulombic term.

Note that these potentials are related to the Buckingham potential.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- A (energy units)
- rho (distance units)
- sigma (distance units)
- C (energy units * distance units^6)
- D (energy units * distance units^8)
- cutoff (distance units)

The second coefficient, rho, must be greater than zero.

The last coefficient is optional. If not specified, the global A,C,D cutoff specified in the *pair_style* command is used.

For *buck/coul/long* and *born/coul/wolf* no Coulombic cutoff can be specified for an individual IJ type pair. All type pairs use the same global Coulombic cutoff specified in the *pair_style* command.
Styles with a \textit{cuda}, \textit{gpu}, \textit{omp}, or \textit{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section\_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \texttt{-suffix} command-line switch when you invoke LAMMPS, or you can use the \texttt{suffix} command in your input script.

See Section\_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

\underline{Mixing, shift, table, tail correction, restart, rRESPA info:}

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These styles support the \texttt{pair\_modify} shift option for the energy of the \texttt{exp()}, \texttt{1/r}^6, and \texttt{1/r}^8 portion of the pair interaction.

The \texttt{born/coul/long} pair style does not support the \texttt{pair\_modify} table option since a tabulation capability has not yet been added to this potential.

These styles support the \texttt{pair\_modify tail} option for adding long-range tail corrections to energy and pressure.

These styles writes their information to binary restart files, so \texttt{pair\_style} and \texttt{pair\_coeff} commands do not need to be specified in an input script that reads a restart file.

These styles can only be used via the \texttt{pair} keyword of the \texttt{run\_style respa} command. They do not support the \texttt{inner, middle, outer} keywords.

\underline{Restrictions:}

The \texttt{born/coul/long} style is part of the KSPACE package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

\underline{Related commands:}

\texttt{pair\_coeff, pair\_style buck}

\underline{Default:} none

pair_style brownian command

pair_style brownian/omp command

pair_style brownian/poly command

pair_style brownian/poly/omp command

Syntax:

pair_style style mu flaglog flagfld cutinner cutoff t_target seed flagHI flagVF

- style = brownian or brownian/poly
- mu = dynamic viscosity (dynamic viscosity units)
- flaglog = 0/1 log terms in the lubrication approximation on/off
- flagfld = 0/1 to include/exclude Fast Lubrication Dynamics effects
- cutinner = inner cutoff distance (distance units)
- cutoff = outer cutoff for interactions (distance units)
- t_target = target temp of the system (temperature units)
- seed = seed for the random number generator (positive integer)
- flagHI (optional) = 0/1 to include/exclude 1/r hydrodynamic interactions
- flagVF (optional) = 0/1 to include/exclude volume fraction corrections in the long-range isotropic terms

Examples:

pair_style brownian 1.5 1 1 2.01 2.5 2.0 5878567 (assuming radius = 1)
pair_coeff 1 1 2.05 2.8
pair_coeff * *

Description:

Styles brownian and brownain/poly compute Brownian forces and torques on finite-size particles. The former requires monodisperse spherical particles; the latter allows for polydisperse spherical particles.

These pair styles are designed to be used with either the pair_style lubricate or pair_style lubricateU commands to provide thermostatting when dissipative lubrication forces are acting. Thus the parameters mu, flaglog, flagfld, cutinner, and cutoff should be specified consistent with the settings in the lubrication pair styles. For details, refer to either of the lubrication pair styles.

The t_target setting is used to specify the target temperature of the system. The random number seed is used to generate random numbers for the thermostatting procedure.

The flagHI and flagVF settings are optional. Neither should be used, or both must be defined.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- cutinner (distance units)
- cutoff (distance units)
The two coefficients are optional. If neither is specified, the two cutoffs specified in the pair_style command are used. Otherwise both must be specified.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in this section of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See this section of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the two cutoff distances for this pair style can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

These styles are part of the FLD package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Only spherical monodisperse particles are allowed for pair_style brownian.

Only spherical particles are allowed for pair_style brownian/poly.

Related commands:

pair_coeff, pair_style lubricate, pair_style lubricateU

Default:

The default settings for the optional args are flagHI = 1 and flagVF = 1.
pair_style buck command
pair_style buck/cuda command
pair_style buck/gpu command
pair_style buck/omp command
pair_style buck/coul/cut command
pair_style buck/coul/cut/cuda command
pair_style buck/coul/cut/gpu command
pair_style buck/coul/cut/omp command
pair_style buck/coul/long command
pair_style buck/coul/long/cuda command
pair_style buck/coul/long/gpu command
pair_style buck/coul/long/omp command

Syntax:

pair_style style args

style = buck or buck/coul/cut or buck/coul/long
args = list of arguments for a particular style

buck args = cutoff
cutoff = global cutoff for Buckingham interactions (distance units)
buck/coul/cut args = cutoff (cutoff2)
cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg) (distance units)
cutoff2 = global cutoff for Coulombic (optional) (distance units)
buck/coul/long args = cutoff (cutoff2)
cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg) (distance units)
cutoff2 = global cutoff for Coulombic (optional) (distance units)

Examples:

pair_style buck 2.5
pair_coeff * * 100.0 1.5 200.0
pair_coeff * * 100.0 1.5 200.0 3.0

pair_style buck/coul/cut 10.0
pair_style buck/coul/cut 10.0 8.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff 1 1 100.0 1.5 200.0 9.0
Description:

The *buck* style computes a Buckingham potential (exp/6 instead of Lennard-Jones 12/6) given by

\[
E = Ae^{-r/\rho} - \frac{C}{r^6} \quad r < r_c
\]

where \( \rho \) is an ionic-pair dependent length parameter, and \( r_c \) is the cutoff.

The *buck/coul/cut* and *buck/coul/long* styles add a Coulombic term as described for the *lj/cut* pair styles. For *buck/coul/long*, an additional damping factor is applied to the Coulombic term so it can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

If one cutoff is specified for the *born/coul/cut* and *born/coul/long* styles, it is used for both the A,C and Coulombic terms. If two cutoffs are specified, the first is used as the cutoff for the A,C terms, and the second is the cutoff for the Coulombic term.

Note that these potentials are related to the Born-Mayer-Huggins potential.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- A (energy units)
- \( \rho \) (distance units)
- C (energy-distance^6 units)
- cutoff (distance units)
- cutoff2 (distance units)

The second coefficient, \( \rho \), must be greater than zero.

The latter 2 coefficients are optional. If not specified, the global A,C and Coulombic cutoffs are used. If only one cutoff is specified, it is used as the cutoff for both A,C and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the A,C and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *buck*, since it has no Coulombic terms.

For *buck/coul/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual IJ type pair. All type pairs use the same global Coulombic cutoff specified in the *pair_style* command.

Styles with a *cuda*, *gpu*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for
round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These styles support the pair_modify shift option for the energy of the exp() and 1/r^6 portion of the pair interaction.

The buck/coul/long pair style does not support the pair_modify table option since a tabulation capability has not yet been added to this potential.

These styles support the pair_modify tail option for adding long-range tail corrections to energy and pressure for the A,C terms in the pair interaction.

These styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These styles can only be used via the pair keyword of the run_style respa command. They do not support the inner, middle, outer keywords.

Restrictions:

The buck/coul/long style is part of the KSPACE package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style born

Default: none
pair_style buck/coul command

pair_style buck/coul/omp command

Syntax:

pair_style buck/coul flag_buck flag_coul cutoff (cutoff2)

- **flag_buck** = long or cut
  - long = use Kspace long-range summation for the dispersion term 1/r^6
  - cut = use a cutoff
- **flag_coul** = long or off
  - long = use Kspace long-range summation for the Coulombic term 1/r
  - off = omit the Coulombic term
- **cutoff** = global cutoff for Buckingham (and Coulombic if only 1 cutoff) (distance units)
- **cutoff2** = global cutoff for Coulombic (optional) (distance units)

Examples:

pair_style buck/coul cut off 2.5
pair_style buck/coul cut long 2.5 4.0
pair_style buck/coul long long 2.5 4.0
pair_coeff * * 1 1
pair_coeff 1 1 1 3 4

Description:

The buck/coul style computes a Buckingham potential (exp/6 instead of Lennard-Jones 12/6) and Coulombic potential, given by

\[ E = Ae^{-r/\rho} - \frac{C}{r^6} \quad r < r_c \]

\[ E = \frac{Cq_iq_j}{er} \quad r < r_c \]

\( r_c \) is the cutoff. If one cutoff is specified in the pair_style command, it is used for both the Buckingham and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the Buckingham and Coulombic terms respectively.

The purpose of this pair style is to capture long-range interactions resulting from both attractive 1/r^6 Buckingham and Coulombic 1/r interactions. This is done by use of the flag_buck and flag_coul settings. The "Ismail" paper has more details on when it is appropriate to include long-range 1/r^6 interactions, using this...
potential.

If flag_buck is set to long, no cutoff is used on the Buckingham 1/r^6 dispersion term. The long-range portion is calculated by using the kspace_style ewald/n command. The specified Buckingham cutoff then determines which portion of the Buckingham interactions are computed directly by the pair potential versus which part is computed in reciprocal space via the Kspace style. If flag_buck is set to cut, the Buckingham interactions are simply cutoff, as with pair_style buck.

If flag_coul is set to long, no cutoff is used on the Coulombic interactions. The long-range portion is calculated by using any style, including ewald/n of the kspace_style command. Note that if flag_buck is also set to long, then only the ewald/n Kspace style can perform the long-range calculations for both the Buckingham and Coulombic interactions. If flag_coul is set to off, Coulombic interactions are not computed.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A (energy units)
- rho (distance units)
- C (energy-distance^6 units)
- cutoff (distance units)
- cutoff2 (distance units)

The second coefficient, rho, must be greater than zero.

The latter 2 coefficients are optional. If not specified, the global Buckingham and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both Buckingham and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the Buckingham and Coulombic cutoffs for this type pair. Note that if you are using flag_buck set to long, you cannot specify a Buckingham cutoff for an atom type pair, since only one global Buckingham cutoff is allowed. Similarly, if you are using flag_coul set to long, you cannot specify a Coulombic cutoff for an atom type pair, since only one global Coulombic cutoff is allowed.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair styles does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This pair style supports the pair_modify shift option for the energy of the exp() and 1/r^6 portion of the pair interaction, assuming flag_buck is cut.
This pair style does not support the `pair_modify` shift option for the energy of the Buckingham portion of the pair interaction.

This pair style does not support the `pair_modify` table option since a tabulation capability has not yet been added to this potential.

This pair style write its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style supports the use of the `inner`, `middle`, and `outer` keywords of the `run_style respa` command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the `run_style` command for details.

**Restrictions:**

This style is part of the USER-EWALDN package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

`pair_coeff`

**Default:** none

(Ismail) Ismail, Tsige, In ‘t Veld, Grest, Molecular Physics (accepted) (2007).
pair_style lj/charmm/coul/charmm command
pair_style lj/charmm/coul/charmm/cuda command
pair_style lj/charmm/coul/charmm/omp command
pair_style lj/charmm/coul/charmm/implicit command
pair_style lj/charmm/coul/charmm/implicit/cuda command
pair_style lj/charmm/coul/charmm/implicit/omp command
pair_style lj/charmm/coul/long command
pair_style lj/charmm/coul/long/cuda command
pair_style lj/charmm/coul/long/gpu command
pair_style lj/charmm/coul/long/opt command
pair_style lj/charmm/coul/long/omp command
pair_style lj/charmm/coul/pppm/omp command

Syntax:

pair_style style args

- style = lj/charmm/coul/charmm or lj/charmm/coul/charmm/implicit or lj/charmm/coul/long
- args = list of arguments for a particular style

\texttt{lj/charmm/coul/charmm} args = inner outer (inner2) (outer2)
  inner, outer = global switching cutoffs for Lennard Jones (and Coulombic if only 2 args)
  inner2, outer2 = global switching cutoffs for Coulombic (optional)
\texttt{lj/charmm/coul/charmm/implicit} args = inner outer (inner2) (outer2)
  inner, outer = global switching cutoffs for LJ (and Coulombic if only 2 args)
  inner2, outer2 = global switching cutoffs for Coulombic (optional)
\texttt{lj/charmm/coul/long} args = inner outer (cutoff)
  inner, outer = global switching cutoffs for LJ (and Coulombic if only 2 args)
  cutoff = global cutoff for Coulombic (optional, outer is Coulombic cutoff if only 2 args)

Examples:

pair_style lj/charmm/coul/charmm 8.0 10.0
pair_style lj/charmm/coul/charmm 8.0 10.0 7.0 9.0
pair_coeff * * 100.0 2.0
pair_coeff 1 1 100.0 2.0 150.0 3.5

pair_style lj/charmm/coul/charmm/implicit 8.0 10.0
pair_style lj/charmm/coul/charmm/implicit 8.0 10.0 7.0 9.0
Description:

The *lj/charmm* styles compute LJ and Coulombic interactions with an additional switching function \( S(r) \) that ramps the energy and force smoothly to zero between an inner and outer cutoff. It is a widely used potential in the CHARMM MD code. See (MacKerell) for a description of the CHARMM force field.

\[
E = \begin{cases} 
LJ(r) & r < r_{\text{in}} \\
S(r) \times LJ(r) & r_{\text{in}} < r < r_{\text{out}} \\
0 & r > r_{\text{out}}
\end{cases}
\]

\[
LJ(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]
\]

\[
C(r) = \frac{Cq_i q_j}{\epsilon r}
\]

\[
S(r) = \frac{[r_{\text{out}}^2 - r^2]^2 [r_{\text{out}}^2 + 2r^2 - 3r_{\text{in}}^2]}{[r_{\text{out}}^2 - r_{\text{in}}^2]^3}
\]

Both the LJ and Coulombic terms require an inner and outer cutoff. They can be the same for both formulas or different depending on whether 2 or 4 arguments are used in the pair_style command. In each case, the inner cutoff distance must be less than the outer cutoff. It is typical to make the difference between the 2 cutoffs about 1.0 Angstrom.

Style *lj/charmm/coul/charmm/implicit* computes the same formulas as style *lj/charmm/coul/charmm* except that an additional \( 1/r \) term is included in the Coulombic formula. The Coulombic energy thus varies as \( 1/r^2 \). This is effectively a distance-dependent dielectric term which is a simple model for an implicit solvent with additional screening. It is designed for use in a simulation of an unsolvated biomolecule (no explicit water molecules).

Styles *lj/charmm/coul/long* and *lj/charmm/coul/pppm/omp* compute the same formulas as style *lj/charmm/coul/charmm* except that an additional damping factor is applied to the Coulombic term, as in the discussion for pair style *lj/cut/coul/long*. Only one Coulombic cutoff is specified for *lj/charmm/coul/long*; if only 2 arguments are used in the pair_style command, then the outer LJ cutoff is used as the single Coulombic cutoff.
Style \textit{lj/charmm/coul/pppm/omp} is a variant for use with K-space style \textit{pppm/proxy} and OpenMP multi-threading and will perform the corresponding reciprocal space calculation concurrently with the pair calculation in a separate thread. For certain parallel setups, this may have a performance benefit over performing k-space style and pair style separately and one after the other.

The following coefficients must be defined for each pair of atoms types via the \texttt{pair\_coeff} command as in the examples above, or in the data file or restart files read by the \texttt{read\_data} or \texttt{read\_restart} commands, or by mixing as described below:

- \texttt{epsilon} (energy units)
- \texttt{sigma} (distance units)
- \texttt{epsilon\_14} (energy units)
- \texttt{sigma\_14} (distance units)

Note that \texttt{sigma} is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at $2^{(1/6)} \sigma$.

The latter 2 coefficients are optional. If they are specified, they are used in the LJ formula between 2 atoms of these types which are also first and fourth atoms in any dihedral. No cutoffs are specified because this CHARMM force field does not allow varying cutoffs for individual atom pairs; all pairs use the global cutoff(s) specified in the \texttt{pair\_style} command.

Styles with a \texttt{cuda}, \texttt{gpu}, \texttt{omp}, or \texttt{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section \texttt{accelerate} of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \texttt{-suffix} command-line switch when you invoke LAMMPS, or you can use the \texttt{suffix} command in your input script.

See Section \texttt{accelerate} of the manual for more instructions on how to use the accelerated styles effectively.

\textbf{Mixing, shift, table, tail correction, restart, rRESPA info:}

For atom type pairs I,J and I \neq J, the \texttt{epsilon}, \texttt{sigma}, \texttt{epsilon\_14}, and \texttt{sigma\_14} coefficients for all of the \textit{lj/charmm} pair styles can be mixed. The default mix value is \texttt{arithmetic} to coincide with the usual settings for the CHARMM force field. See the "pair\_modify" command for details.

None of the \textit{lj/charmm} pair styles support the \texttt{pair\_modify} shift option, since the Lennard-Jones portion of the pair interaction is smoothed to 0.0 at the cutoff.

The \textit{lj/charmm/coul/long} style supports the \texttt{pair\_modify} table option since it can tabulate the short-range portion of the long-range Coulombic interaction.

None of the \textit{lj/charmm} pair styles support the \texttt{pair\_modify} tail option for adding long-range tail corrections to energy and pressure, since the Lennard-Jones portion of the pair interaction is smoothed to 0.0 at the cutoff.
All of the lj/charmm pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The lj/charmm/coul/long pair style supports the use of the inner, middle, and outer keywords of the run_style respa command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. The other styles only support the pair keyword of run_style respa. See the run_style command for details.

Restrictions:

The lj/charmm/coul/charmm and lj/charmm/coul/charmm/implicit styles are part of the MOLECULE package. The lj/charmm/coul/long style is part of the KSPACE package. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info. Note that the MOLECULE and KSPACE packages are installed by default.

Related commands:

pair_coeff

Default: none

pair_style lj/class2 command

pair_style lj/class2/cuda command

pair_style lj/class2/gpu command

pair_style lj/class2/omp command

pair_style lj/class2/coul/cut command

pair_style lj/class2/coul/cut/cuda command

pair_style lj/class2/coul/cut/omp command

pair_style lj/class2/coul/long command

pair_style lj/class2/coul/long/cuda command

pair_style lj/class2/coul/long/gpu command

pair_style lj/class2/coul/long/omp command

pair_style lj/class2/coul/pppm/omp command

Syntax:

pair_style style args

- style = lj/class2 or lj/class2/coul/cut or lj/class2/coul/long
- args = list of arguments for a particular style

lj/class2 args = cutoff
- cutoff = global cutoff for class 2 interactions (distance units)

lj/class2/coul/cut args = cutoff (cutoff2)
- cutoff = global cutoff for class 2 (and Coulombic if only 1 arg) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

lj/class2/coul/long args = cutoff (cutoff2)
- cutoff = global cutoff for class 2 (and Coulombic if only 1 arg) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

Examples:

pair_style lj/class2 10.0
pair_coeff * * 100.0 2.5
pair_coeff 1 2* 100.0 2.5 9.0

pair_style lj/class2/coul/cut 10.0
pair_style lj/class2/coul/cut 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
pair_coeff 1 1 100.0 3.5 9.0 9.0
pair_style lj/class2/coul/long 10.0
pair_style lj/class2/coul/long 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0

**Description:**

The *lj/class2* styles compute a 6/9 Lennard-Jones potential given by

\[
E = \epsilon \left[ 2 \left( \frac{\sigma}{r} \right)^9 - 3 \left( \frac{\sigma}{r} \right)^6 \right] \quad r < r_c
\]

\(r_c\) is the cutoff.

The *lj/class2/coul/cut* and *lj/class2/coul/long* styles add a Coulombic term as described for the *lj/cut* pair styles.

See (Sun) for a description of the COMPASS class2 force field.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- \(\epsilon\) (energy units)
- \(\sigma\) (distance units)
- \(cutoff1\) (distance units)
- \(cutoff2\) (distance units)

The latter 2 coefficients are optional. If not specified, the global class 2 and Coulombic cutoffs are used. If only one cutoff is specified, it is used as the cutoff for both class 2 and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the class 2 and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *lj/class2*, since it has no Coulombic terms.

For *lj/class2/coul/long* only the class 2 cutoff can be specified since a Coulombic cutoff cannot be specified for an individual \(IJ\) type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

If the pair_coeff command is not used to define coefficients for a particular \(I \neq J\) type pair, the mixing rule for \(\epsilon\) and \(\sigma\) for all class2 potentials is to use the *sixthpower* formulas documented by the pair_modify command. The pair_modify mix setting is thus ignored for class2 potentials for \(\epsilon\) and \(\sigma\). However it is still followed for mixing the cutoff distance.

**Styles:**

Styles with a *cuda*, *gpu*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.
You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/class2 pair styles can be mixed. Epsilon and sigma are always mixed with the value sixthpower. The cutoff distance is mixed by whatever option is set by the pair_modify command (default = geometric). See the "pair_modify" command for details.

All of the lj/class2 pair styles support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction.

The lj/class2/coul/long pair style does not support the pair_modify table option since a tabulation capability has not yet been added to this potential.

All of the lj/class2 pair styles support the pair_modify tail option for adding a long-range tail correction to the energy and pressure of the Lennard-Jones portion of the pair interaction.

All of the lj/class2 pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

All of the lj/class2 pair styles can only be used via the pair keyword of the run_style respa command. They do not support the inner, middle, outer keywords.

**Restrictions:**

These styles are part of the CLASS2 package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

pair_coeff

Default: none

pair_coeff command

Syntax:

pair_coeff I J args

- I,J = atom types (see asterisk form below)
- args = coefficients for one or more pairs of atom types

Examples:

pair_coeff 1 2 1.0 1.0 2.5
pair_coeff 2 * 1.0 1.0
pair_coeff 3* 1*2 1.0 1.0 2.5
pair_coeff * * 1.0 1.0
pair_coeff * * nialhjnea 1 1 2
pair_coeff * 3 morse.table ENTRY1
pair_coeff 1 2 lj/cut 1.0 1.0 2.5 (for pair_style hybrid)

Description:

Specify the pairwise force field coefficients for one or more pairs of atom types. The number and meaning of the coefficients depends on the pair style. Pair coefficients can also be set in the data file read by the read_data command or in a restart file.

I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values.

A wildcard asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

Note that a pair_coeff command can override a previous setting for the same I,J pair. For example, these commands set the coeffs for all I,J pairs, then overwrite the coeffs for just the I,J = 2,3 pair:

pair_coeff * * 1.0 1.0 2.5
pair_coeff 2 3 2.0 1.0 1.12

A line in a data file that specifies pair coefficients uses the exact same format as the arguments of the pair_coeff command in an input script, with the exception of the I,J type arguments. In each line of the “Pair Coeffs” section of a data file, only a single type I is specified, which sets the coefficients for type I interacting with type I. This is because the section has exactly N lines, where N = the number of atom types. For this reason, the wild-card asterisk should also not be used as part of the I argument. Thus in a data file, the line corresponding to the 1st example above would be listed as

2 1.0 1.0 2.5

For many potentials, if coefficients for type pairs with I != J are not set explicitly by a pair_coeff command, the values are inferred from the I,I and J,J settings by mixing rules; see the pair_modify command for a discussion.
Details on this option as it pertains to individual potentials are described on the doc page for the potential.

Here is an alphabetic list of pair styles defined in LAMMPS. Click on the style to display the formula it computes, arguments specified in the pair_style command, and coefficients specified by the associated pair_coeff command.

Note that there are also additional pair styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the pair section of this page.

There are also additional accelerated pair styles included in the LAMMPS distribution for faster performance on CPUs and GPUs. The list of these with links to the individual styles are given in the pair section of this page.

- **pair_style hybrid** - multiple styles of pairwise interactions
- **pair_style hybrid/overlay** - multiple styles of superposed pairwise interactions
- **pair_style adp** - angular dependent potential (ADP) of Mishin
- **pair_style airebo** - AIREBO potential of Stuart
- **pair_style bop** - BOP potential of Pettifor
- **pair_style born** - Born-Mayer-Huggins potential
- **pair_style born/coul/long** - Born-Mayer-Huggins with long-range Coulombics
- **pair_style born/coul/wolf** - Born-Mayer-Huggins with Coulombics via Wolf potential
- **pair_style brownian** - Brownian potential for Fast Lubrication Dynamics
- **pair_style brownian/poly** - Brownian potential for Fast Lubrication Dynamics with polydispersity
- **pair_style buck** - Buckingham potential
- **pair_style buck/coul/cut** - Buckingham with cutoff Coulomb
- **pair_style buck/coul/long** - Buckingham with long-range Coulomb
- **pair_style colloid** - integrated colloidal potential
- **pair_style comb** - charge-optimized many-body (COMB) potential
- **pair_style coul/cut** - cutoff Coulombic potential
- **pair_style coul/debye** - cutoff Coulombic potential with Debye screening
- **pair_style coul/long** - long-range Coulombic potential
- **pair_style coul/wolf** - Coulombics via Wolf potential
- **pair_style dipole/cut** - point dipoles with cutoff
- **pair_style dpd** - dissipative particle dynamics (DPD)
- **pair_style dpd/tstat** - DPD thermostatting
- **pair_style dsmc** - Direct Simulation Monte Carlo (DSMC)
- **pair_style eam** - embedded atom method (EAM)
- **pair_style eam/alloy** - alloy EAM
- **pair_style eam/fs** - Finnis-Sinclair EAM
- **pair_style eim** - embedded ion method (EIM)
- **pair_style gauss** - Gaussian potential
- **pair_style gayberne** - Gay-Berne ellipsoidal potential
- **pair_style gran/hertz/history** - granular potential with Hertzian interactions
- **pair_style gran/hooke** - granular potential with history effects
- **pair_style gran/hooke/history** - granular potential without history effects
- **pair_style hbond/dreiding/lj** - DREIDING hydrogen bonding LJ potential
- **pair_style hbond/dreiding/morse** - DREIDING hydrogen bonding Morse potential
- **pair_style lcbop** - long-range bond-order potential (LCBOP)
- **pair_style line/lj** - LJ potential between line segments
- **pair_style lj/charmm/coul/charmm** - CHARMM potential with cutoff Coulomb
- **pair_style lj/charmm/coul/charmm/implicit** - CHARMM for implicit solvent
- **pair_style lj/charmm/coul/long** - CHARMM with long-range Coulomb
- **pair_style lj/class2** - COMPASS (class 2) force field with no Coulomb
• pair_style lj/class2/coul/cut - COMPASS with cutoff Coulomb
• pair_style lj/class2/coul/long - COMPASS with long-range Coulomb
• pair_style lj/cut - cutoff Lennard-Jones potential with no Coulomb
• pair_style lj/cut/coul/cut - LJ with cutoff Coulomb
• pair_style lj/cut/coul/debye - LJ with Debye screening added to Coulomb
• pair_style lj/cut/coul/long - LJ with long-range Coulomb
• pair_style lj/cut/coul/long/tip4p - LJ with long-range Coulomb for TIP4P water
• pair_style lj/expand - Lennard-Jones for variable size particles
• pair_style lj/gromacs - GROMACS-style Lennard-Jones potential
• pair_style lj/gromacs/coul/gromacs - GROMACS-style LJ and Coulombic potential
• pair_style lj/smooth/lj - smoothed Lennard-Jones potential
• pair_style lj/smooth/linear - linear smoothed Lennard-Jones potential
• pair_style lj96/cut - Lennard-Jones 9/6 potential
• pair_style lubricate - hydrodynamic lubrication forces
• pair_style lubricate/poly - hydrodynamic lubrication forces with polydispersity
• pair_style lubricateU - hydrodynamic lubrication forces for Fast Lubrication Dynamics
• pair_style lubricateU/poly - hydrodynamic lubrication forces for Fast Lubrication Dynamics with polydispersity
• pair_style meam - modified embedded atom method (MEAM)
• pair_style morse - Morse potential
• pair_style peri/lps - peridynamic LPS potential
• pair_style peri/pmb - peridynamic PMB potential
• pair_style reax - ReaxFF potential
• pair_style rebo - 2nd-generation REBO potential of Brenner
• pair_style resquared - Everaers RE-Squared ellipsoidal potential
• pair_style soft - Soft (cosine) potential
• pair_style sw - Stillinger-Weber 3-body potential
• pair_style table - tabulated pair potential
• pair_style tersoff - Tersoff 3-body potential
• pair_style tersoff/zbl - Tersoff/ZBL 3-body potential
• pair_style tri/lj - LJ potential between triangles
• pair_style yukawa - Yukawa potential
• pair_style yukawa/colloid - screened Yukawa potential for finite-size particles

Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

Related commands:

pair_style, pair_modify, read_data, read_restart, pair_write

Default: none
pair_style colloid command

pair_style colloid/gpu command

pair_style colloid/omp command

Syntax:

pair_style colloid cutoff

  * cutoff = global cutoff for colloidal interactions (distance units)

Examples:

pair_style colloid 10.0
pair_coeff * * 25 1.0 10.0 10.0
pair_coeff 1 1 144 1.0 0.0 0.0 3.0
pair_coeff 1 2 75.398 1.0 0.0 10.0 9.0
pair_coeff 2 2 39.478 1.0 10.0 10.0 25.0

Description:

Style colloid computes pairwise interactions between large colloidal particles and small solvent particles using 3 formulas. A colloidal particle has a size > sigma; a solvent particle is the usual Lennard-Jones particle of size sigma.

The colloid-colloid interaction energy is given by
\[ U_A = -\frac{A_{cc}}{6} \left[ \frac{2a_1a_2}{r^2 - (a_1 + a_2)^2} + \frac{2a_1a_2}{r^2 - (a_1 - a_2)^2} + \ln \left( \frac{r^2 - (a_1 + a_2)^2}{r^2 - (a_1 - a_2)^2} \right) \right] \]

\[ U_R = \frac{A_{cc}}{37800} \frac{\sigma^6}{r} \left[ \frac{r^2 - 7r(a_1 + a_2) + 6(a_1^2 + 7a_1a_2 + a_2^2)}{(r - a_1 - a_2)^7} \right. \\
\left. + \frac{r^2 + 7r(a_1 + a_2) + 6(a_1^2 + 7a_1a_2 + a_2^2)}{(r + a_1 + a_2)^7} \right. \\
\left. - \frac{r^2 + 7r(a_1 - a_2) + 6(a_1^2 - 7a_1a_2 + a_2^2)}{(r + a_1 - a_2)^7} \right. \\
\left. - \frac{r^2 - 7r(a_1 - a_2) + 6(a_1^2 - 7a_1a_2 + a_2^2)}{(r - a_1 + a_2)^7} \right] \]

\[ U = U_A + U_R, \quad r < r_c \]

where \( A_{cc} \) is the Hamaker constant, \( a_1 \) and \( a_2 \) are the radii of the two colloidal particles, and \( R_c \) is the cutoff. This equation results from describing each colloidal particle as an integrated collection of Lennard-Jones particles of size \( \sigma \) and is derived in (Everaers).

The colloid-solvent interaction energy is given by

\[ U = \frac{2a^3 \sigma^3 A_{cs}}{9(a^2 - r^2)^3} \left[ 1 - \frac{(5a^6 + 45a^4r^2 + 63a^2r^4 + 15r^6}\sigma^6}{\frac{15(a - r)^6(a + r)^6}} \right], \quad r < r_c \]

where \( A_{cs} \) is the Hamaker constant, \( a \) is the radius of the colloidal particle, and \( R_c \) is the cutoff. This formula is derived from the colloid-colloid interaction, letting one of the particle sizes go to zero.

The solvent-solvent interaction energy is given by the usual Lennard-Jones formula.
with $A_{ss}$ set appropriately, which results from letting both particle sizes go to zero.

When used in combination with `pair_style yukawa/colloid`, the two terms become the so-called DLVO potential, which combines electrostatic repulsion and van der Waals attraction.

The following coefficients must be defined for each pair of atoms types via the `pair_coeff` command as in the examples above, or in the data file or restart files read by the `read_data` or `read_restart` commands, or by mixing as described below:

- $A$ (energy units)
- $\sigma$ (distance units)
- $d_1$ (distance units)
- $d_2$ (distance units)
- cutoff (distance units)

$A$ is the Hamaker energy prefactor and should typically be set as follows:

- $A_{cc} = \text{colloid/colloid} = 4 \pi^2 = 39.5$
- $A_{cs} = \text{colloid/solvent} = \sqrt{A_{cc}A_{ss}}$
- $A_{ss} = \text{solvent/solvent} = 144$ (assuming $\epsilon = 1$, so that $144/36 = 4$)

Sigma is the size of the solvent particle or the constituent particles integrated over in the colloidal particle and should typically be set as follows:

- $\Sigma_{cc} = \text{colloid/colloid} = 1.0$
- $\Sigma_{cs} = \text{colloid/solvent} = \text{arithmetic mixing between colloid sigma and solvent sigma}$
- $\Sigma_{ss} = \text{solvent/solvent} = 1.0$ or whatever size the solvent particle is

Thus typically $\Sigma_{cs} = 1.0$, unless the solvent particle's size $\neq 1.0$.

$d_1$ and $d_2$ are particle diameters, so that $d_1 = 2a_1$ and $d_2 = 2a_2$ in the formulas above. Both $d_1$ and $d_2$ must be values $\geq 0$. If $d_1 > 0$ and $d_2 > 0$, then the pair interacts via the colloid-colloid formula above. If $d_1 = 0$ and $d_2 = 0$, then the pair interacts via the solvent-solvent formula. I.e. a $d$ value of 0 is a Lennard-Jones particle of size $\sigma$. If either $d_1 = 0$ or $d_2 = 0$ and the other is larger, then the pair interacts via the colloid-solvent formula.

Note that the diameter of a particular particle type may appear in multiple `pair_coeff` commands, as it interacts with other particle types. You should insure the particle diameter is specified consistently each time it appears.

The last coefficient is optional. If not specified, the global cutoff specified in the `pair_style` command is used. However, you typically want different cutoffs for interactions between different particle sizes. E.g. if colloidal particles of diameter 10 are used with solvent particles of diameter 1, then a solvent-solvent cutoff of 2.5 would correspond to a colloid-colloid cutoff of 25. A good rule-of-thumb is to use a colloid-solvent cutoff that is half the big diameter + 4 times the small diameter. I.e. $9 = 5 + 4$ for the colloid-solvent cutoff in this case.

IMPORTANT NOTE: When using `pair_style colloid` for a mixture with 2 (or more) widely different particles sizes (e.g. sigma=10 colloids in a background sigam=1 LJ fluid), you will likely want to use these commands for
efficiency: neighbor multi and communicate multi.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A, sigma, d1, and d2 coefficients and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. D1 and d2 are distance values and are mixed like sigma. The default mix value is geometric. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This style is part of the COLLOID package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Normally, this pair style should be used with finite-size particles which have a diameter, e.g. see the atom_style sphere command. However, this is not a requirement, since the only definition of particle size is via the pair_coeff parameters for each type. In other words, the physical radius of the particle is ignored. Thus you should insure that the d1,d2 parameters you specify are consistent with the physical size of the particles of that type.

Per-particle polydispersity is not yet supported by this pair style; only per-type polydispersity is enabled via the pair_coeff parameters.

Related commands:

pair_coeff
pair_style comb command

pair_style comb/omp command

Syntax:

pair_style comb

Examples:

pair_style comb
pair_coeff * * ../potentials/ffield.comb Si
pair_coeff * * ../potentials/ffield.comb Hf Si O

Description:

Style `comb` computes a variable charge COMB (Charge-Optimized Many-Body) potential as described in (COMB_1) and (COMB_2). The energy \( E \) of a system of atoms is given by

\[
E_T = \sum_i E_i^S + \frac{1}{2} \sum_{i \neq j} V_{ij}(r_{ij}, q_i, q_j) + E_i^{BB}
\]

\[
V_{ij}(r_{ij}, q_i, q_j) = U_{ij}^R(r_{ij}) + U_{ij}^A(r_{ij}, q_i, q_j) + U_{ij}^I(r_{ij}, q_i, q_j) + U_{ij}^V(r_{ij})
\]

where \( E_T \) is the total potential energy of the system, \( E_i^S \) is the self-energy term of atom \( i \), \( V_{ij} \) is the interatomic potential between the \( i \)th and \( j \)th atoms, \( r_{ij} \) is the distance of the atoms \( i \) and \( j \), and \( q_i \) and \( q_j \) are charges of the atoms, and \( E_i^{BB} \) is the bond-bending term of atom \( i \).

The interatomic potential energy \( V_{ij} \) consists of four components: two-body short-range repulsion, \( U_{ij}^R \), many-body short-range attraction, \( U_{ij}^A \), long-range Coulombic electrostatic interaction, \( U_{ij}^I \), and van der Waals energy, \( U_{ij}^V \), which are defined as:

\[
U_{ij}^R(r_{ij}) = f_{S_{ij}} A_{ij} \exp(-\lambda_{ij} r_{ij})
\]

\[
U_{ij}^A(r_{ij}, q_i, q_j) = -f_{S_{ij}} b_{ij} B_{ij} \exp(-\alpha_{ij} r_{ij})
\]

\[
U_{ij}^I(r_{ij}, q_i, q_j) = J_{ij}(r_{ij}) q_i q_j
\]

\[
U_{ij}^V(r_{ij}) = f_{L_{ij}} \left( C_{VDW_i} C_{VDW_j} \right)^{\frac{1}{2}} / r_{ij}^6
\]

The short-range repulsion and attraction are based on the Tersoff potential (see the pair_style tersoff command); thus for a zero-charge pure element system with no van der Waals interaction, the COMB potential reduces to Tersoff potential, typically truncated at a short cutoff, e.g. 3 to 4 Angstroms. The long-range Coulombic term uses the Wolf summation method described in Wolf, spherically truncated at a longer cutoff, e.g. 12 Angstroms.
The COMB potential is a variable charge potential. The equilibrium charge on each atom is calculated by the
electron negativity equalization (QEq) method. See Rick for further details. This is implemented by the fix
qeq/comb command, which should normally be specified in the input script when running a model with the
COMB potential. The fix qeq/comb command has options that determine how often charge equilibration is
performed, its convergence criterion, and which atoms are included in the calculation.

Only a single pair_coeff command is used with the comb style which specifies the COMB potential file with
parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional
arguments after the potential file in the pair_coeff command, where N is the number of LAMMPS atom types.
The provided potential file ffield.comb contains all currently-available COMB parameterizations: for Si, Cu, Hf,
Ti, O, their oxides and Zr, Zn and U metals.

For example, if your LAMMPS simulation of a Si/SiO$_2$/HfO$_2$ interface has 4 atom types, and you want the 1st
and last to be Si, the 2nd to be Hf, and the 3rd to be O, and you would use the following pair_coeff command:

```
pair_coeff * * ../potentials/ffield.comb Si Hf O Si
```

The first two arguments must be * * so as to span all LAMMPS atom types. The first and last Si arguments map
LAMMPS atom types 1 and 4 to the Si element in the ffield.comb file. The second Hf argument maps LAMMPS
atom type 2 to the Hf element, and the third O argument maps LAMMPS atom type 3 to the O element in the
potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a
comb potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will
be used with other potentials.

The ffield.comb potential file is in the potentials directory of the LAMMPS distribution. Lines that are not blank
or comments (starting with #) define parameters for a triplet of elements. The 49 parameters in a single entry
correspond to coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2 (the atom bonded to the center atom)
- element 3 (the atom influencing the 1-2 bond in a bond-order sense)
- m
- c
- d
- h (cos_theta0 (can be a value -1 or 1))
- n
- beta
- lambda21, lambda22 of element 1 (1/distance units)
- lambda11, lambda12 of element 1 (1/distance units)
- B of element 1 (energy units)
- A of element 1 (energy units)
- K_LP_1 (energy units, 1st order Legendre polynomial coefficient)
- A123 (cos_theta, theta = equilibrium MOM or OMO bond angles)
- addrep (energy units, additional repulsion)
The parameterization of COMB potentials start with a pure element (e.g. Si, Cu) then extend to its oxide and polymorphs (e.g. SiO₂, Cu₂O). For interactions not involving oxygen (e.g. Si-Cu or Hf-Zr), the COMB potential uses a mixing rule to generate these parameters. For further details on the parameterization and parameters, see the Tersoff doc page and the COMB publications [COMB_1] and [COMB_2]. For more details on 3-body interaction types (e.g. SiSiO vs SiOSi), the mixing rule, and how to generate the potential file, please see the Tersoff doc page.

In the potentials directory, the file *ffield.comb* provides the LAMMPS parameters for COMB's Si, Cu, Ti, Hf and their oxides, as well as pure U, Zn and Zr metals. This file can be used for pure elements (e.g. Si, Zr), binary oxides, binary alloys (e.g. SiCu, TiZr), and complex systems. Note that alloys and complex systems require all 3-body entries be pre-defined in the potential file.

**Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.**

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.
For atom type pairs I,J and I ≠ J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the `pair_modify` shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style, pair_coeff, and fix qeq/comb commands in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the run_style respa command. It does not support the `inner`, `middle`, `outer` keywords.

**Restrictions:**

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair style requires the `newton` setting to be "on" for pair interactions.

The COMB potentials in the `ffield.comb` file provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the COMB potential with any LAMMPS units, but you would need to create your own COMB potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

**Related commands:**

`pair_style`, `pair_coeff`, `fix qeq/comb`

**Default:** none


pair_style coul/cut command

pair_style coul/cut/omp command

pair_style coul/debye command

pair_style coul/debye/omp command

pair_style coul/long command

pair_style coul/long/omp command

pair_style coul/long/gpu command

pair_style coul/wolf command

pair_style coul/wolf/omp command

Syntax:

pair_style coul/cut cutoff
pair_style coul/debye kappa cutoff
pair_style coul/long cutoff
pair_style coul/long/gpu cutoff
pair_style coul/wolf alpha cutoff

- cutoff = global cutoff for Coulombic interactions
- kappa = Debye length (inverse distance units)
- alpha = damping parameter (inverse distance units)

Examples:

pair_style coul/cut 2.5
pair_coeff * *
pair_coeff 2 2 3.5

pair_style coul/debye 1.4 3.0
pair_coeff * *
pair_coeff 2 2 3.5

pair_style coul/long 10.0
pair_coeff * *

pair_style coul/wolf 0.2 9.0
pair_coeff * *

Description:

The *coul/cut* style computes the standard Coulombic interaction potential given by
where $C$ is an energy-conversion constant, $Q_i$ and $Q_j$ are the charges on the 2 atoms, and epsilon is the dielectric constant which can be set by the `dielectric` command. The cutoff $R_c$ truncates the interaction distance.

Style `coul/debye` adds an additional $\exp()$ damping factor to the Coulombic term, given by

$$E = \frac{Cq_i q_j}{\varepsilon r} \exp(-\kappa r) \quad r < R_c$$

where $\kappa$ is the Debye length. This potential is another way to mimic the screening effect of a polar solvent.

Style `coul/wolf` computes Coulombic interactions via the Wolf summation method, described in Wolf, given by:

$$E_i = \frac{1}{2} \sum_{j \neq i} \frac{q_i q_j \text{erfc}(\alpha r_{ij})}{r_{ij}} + \frac{1}{2} \sum_{j \neq i} \frac{q_i q_j \text{erf}(\alpha r_{ij})}{r_{ij}} \quad r < R_c$$

where $\alpha$ is the damping parameter, and $\text{erf}()$ and $\text{erfc}()$ are error-fuction and complementary error-function terms. This potential is essentially a short-range, spherically-truncated, charge-neutralized, shifted, pairwise $1/r$ summation. With a manipulation of adding and subtracting a self term (for $i = j$) to the first and second term on the right-hand-side, respectively, and a small enough $\alpha$ damping parameter, the second term shrinks and the potential becomes a rapidly-converging real-space summation. With a long enough cutoff and small enough $\alpha$ parameter, the energy and forces calculated by the Wolf summation method approach those of the Ewald sum. So it is a means of getting effective long-range interactions with a short-range potential.

Style `coul/long` computes the same Coulombic interactions as style `coul/cut` except that an additional damping factor is applied so it can be used in conjunction with the `kspace_style` command and its `ewald` or `pppm` option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

These potentials are designed to be combined with other pair potentials via the `pair_style hybrid/overlay` command. This is because they have no repulsive core. Hence if they are used by themselves, there will be no repulsion to keep two oppositely charged particles from overlapping each other.

The following coefficients must be defined for each pair of atoms types via the `pair_coeff` command as in the examples above, or in the data file or restart files read by the `read_data` or `read_restart` commands, or by mixing as described below:

- cutoff (distance units)
For `coul/cut` and `coul/debye`, the cutoff coefficient is optional. If it is not used (as in some of the examples above),
the default global value specified in the `pair_style` command is used.

For `coul/long` no cutoff can be specified for an individual I,J type pair via the `pair_coeff` command. All type pairs
use the same global Coulombic cutoff specified in the `pair_style` command.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix.
They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate
of the manual. The accelerated styles take the same arguments and should produce the same results, except for
round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They
are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the
-suffix command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input
script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the cutoff distance for the `coul/cut` style can be mixed. The default mix value is
geometric. See the "pair_modify" command for details.

The `pair_modify` shift option is not relevant for these pair styles.

The `coul/long` style supports the `pair_modify` table option for tabulation of the short-range portion of the
long-range Coulombic interaction.

These pair styles do not support the `pair_modify` tail option for adding long-range tail corrections to energy and
pressure.

These pair styles write their information to binary restart files, so `pair_style` and `pair_coeff` commands do not need
to be specified in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the
`inner`, `middle`, `outer` keywords.

Restrictions:

The `coul/long` style is part of the KSPACE package. It is only enabled if LAMMPS was built with that package
(which it is by default). See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style hybrid/overlay

Default: none

pair_style coul/diel command

Syntax:

pair_style coul/diel cutoff
cutoff = global cutoff (distance units)

Examples:

pair_style coul/diel 3.5
pair_coeff 1 4 78. 1.375 0.112

Description:

Style coul/diel computes a Coulomb correction for implicit solvent ion interactions in which the dielectric permittivity is distance dependent. The dielectric permittivity epsilon_D(r) connects to limiting regimes: One limit is defined by a small dielectric permittivity (close to vacuum) at or close to contact separation between the ions. At larger separations the dielectric permittivity reaches a bulk value used in the regular Coulomb interaction coul/long or coul/cut. The transition is modeled by a hyperbolic function which is incorporated in the Coulomb correction term for small ion separations as follows

\[ E = \frac{Cq_iq_j}{\epsilon r} \left( \frac{\epsilon}{\epsilon_D(r)} - 1 \right) \quad r < r_c \]

\[ \epsilon_D(r) = \frac{5.2 + \epsilon}{2} + \frac{\epsilon - 5.2}{2} \tanh \left( \frac{r - r_{me}}{\sigma_e} \right) \]

where r_me is the inflection point of epsilon_D(r) and sigma_e is a slope defining length scale. C is the same Coulomb conversion factor as in the pair_styles coul/cut, coul/long, and coul/debye. In this way the Coulomb interaction between ions is corrected at small distances r. The lower limit of epsilon_D(r->0)=5.2 due to dielectric saturation (Stiles) while the Coulomb interaction reaches its bulk limit by setting epsilon_D(r->\infty)=epsilon, the bulk value of the solvent which is 78 for water at 298K.

Examples of the use of this type of Coulomb interaction include implicit solvent simulations of salt ions (Lenart) and of ionic surfactants (Jusufi). Note that this potential is only reasonable for implicit solvent simulations and in combination with coul/cut or coul/long. It is also usually combined with gauss/cut, see (Lenart) or (Jusufi).

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- epsilon (no units)
- r_me (distance units)
- sigma_e (distance units)

The global cutoff (r_c) specified in the pair_style command is used.
Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support parameter mixing. Coefficients must be given explicitly for each type of particle pairs.

This pair style supports the pair_modify shift option for the energy of the Gauss-potential portion of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This style is part of the "user-misc" package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff pair_style gauss/cut

Default: none


pair_style dipole/cut command

pair_style dipole/cut/gpu command

pair_style dipole/cut/omp command

pair_style dipole/sf command

pair_style dipole/sf/gpu command

pair_style dipole/sf/omp command

Syntax:

pair_style dipole/cut cutoff (cutoff2)

pair_style dipole/sf cutoff (cutoff2)

- cutoff = global cutoff LJ (and Coulombic if only 1 arg) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

Examples:

pair_style dipole/cut 10.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0

pair_style dipole/sf 9.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0

Description:

Style dipole/cut computes interactions between pairs of particles that each have a charge and/or a point dipole moment. In addition to the usual Lennard-Jones interaction between the particles (Elj) the charge-charge (Eqq), charge-dipole (Eqp), and dipole-dipole (Epp) interactions are computed by these formulas for the energy (E), force (F), and torque (T) between particles I and J.
\[ E_{LJ} = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \]

\[ E_{qq} = \frac{q_i q_j}{r} \]

\[ E_{qp} = \frac{q}{r^3} (p \cdot \vec{r}) \]

\[ E_{pp} = \frac{1}{r^3} (p_i \cdot p_j) - \frac{3}{r^5} (p_i \cdot \vec{r}) (p_j \cdot \vec{r}) \]

\[ F_{qq} = \frac{q_i q_j}{r^3} \vec{r} \]

\[ F_{qp} = -\frac{q}{r^3} \vec{p} + \frac{3q}{r^5} (\vec{p} \cdot \vec{r}) \vec{r} \]

\[ F_{pp} = \frac{3}{r^5} (p_i \cdot p_j) \vec{r} - \frac{15}{r^7} (p_i \cdot \vec{r}) (p_j \cdot \vec{r}) \vec{r} + \frac{3}{r^5} [(p_j \cdot \vec{r}) p_i + (p_i \cdot \vec{r}) p_j] \]

\[ T_{pq} = T_{ij} = \frac{q_j}{r^3} (p_i \times \vec{r}) \]

\[ T_{qp} = T_{ji} = -\frac{q_i}{r^3} (p_j \times \vec{r}) \]

\[ T_{pp} = T_{ij} = -\frac{1}{r^3} (p_i \times p_j) + \frac{3}{r^5} (p_j \cdot \vec{r})(p_i \times \vec{r}) \]

\[ T_{pp} = T_{ji} = -\frac{1}{r^3} (p_j \times p_i) + \frac{3}{r^5} (p_i \cdot \vec{r})(p_j \times \vec{r}) \]

where \( q_i \) and \( q_j \) are the charges on the two particles, \( p_i \) and \( p_j \) are the dipole moment vectors of the two particles, \( r \) is their separation distance, and the vector \( r = R_i - R_j \) is the separation vector between the two particles. Note that \( E_{qq} \) and \( F_{qq} \) are simply Coulombic energy and force, \( F_{ij} = -F_{ji} \) as symmetric forces, and \( T_{ij} \neq -T_{ji} \) since the torques do not act symmetrically. These formulas are discussed in (Allen) and in (Toukmaji).

Style `dipole/sf` computes "shifted-force" interactions between pairs of particles that each have a charge and/or a point dipole moment. In general, a shifted-force potential is a (slightly) modified potential containing extra terms that make both the energy and its derivative go to zero at the cutoff distance; this removes (cutoff-related)
problems in energy conservation and any numerical instability in the equations of motion (Allen). Shifted-force interactions for the Lennard-Jones ($E_{\text{LJ}}$), charge-charge ($E_{\text{qq}}$), charge-dipole ($E_{\text{qp}}$), dipole-charge ($E_{\text{pq}}$) and dipole-dipole ($E_{\text{pp}}$) potentials are computed by these formulas for the energy ($E$), force ($F$), and torque ($T$) between particles I and J:
\[ E_{LJ} = 4\varepsilon \left\{ \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] + \left[ 6 \left( \frac{\sigma}{r_c} \right)^{12} - 3 \left( \frac{\sigma}{r_c} \right)^{6} \right] \left( \frac{r}{r_c} \right)^2 - 7 \left( \frac{\sigma}{r_c} \right)^{12} \right\} \]

\[ E_{qq} = \frac{q_i q_j}{r} \left( 1 - \frac{r}{r_c} \right)^2 \]

\[ E_{pq} = E_{ji} = -\frac{q}{r^3} \left[ 1 - 3 \left( \frac{r}{r_c} \right)^2 + 2 \left( \frac{r}{r_c} \right)^3 \right] (\vec{p} \cdot \vec{r}) \]

\[ E_{qp} = E_{ij} = \frac{q}{r^3} \left[ 1 - 3 \left( \frac{r}{r_c} \right)^2 + 2 \left( \frac{r}{r_c} \right)^3 \right] (\vec{p} \cdot \vec{r}) \]

\[ E_{pp} = \left[ 1 - 4 \left( \frac{r}{r_c} \right)^3 + 3 \left( \frac{r}{r_c} \right)^4 \right] \left[ \frac{1}{r^3} (\vec{p}_i \cdot \vec{p}_j) - \frac{3}{r^5} (\vec{p}_i \cdot \vec{r})(\vec{p}_j \cdot \vec{r}) \right] \]

\[ F_{LJ} = \left\{ \left[ 48\varepsilon \left( \frac{\sigma}{r} \right)^{12} - 24\varepsilon \left( \frac{\sigma}{r} \right)^6 \right] \frac{1}{r^2} - \left[ 48\varepsilon \left( \frac{\sigma}{r_c} \right)^{12} - 24\varepsilon \left( \frac{\sigma}{r_c} \right)^6 \right] \frac{1}{r_c^2} \right\} \vec{r} \]

\[ F_{qq} = \frac{q_i q_j}{r} \left( \frac{1}{r^2} - \frac{1}{r_c^2} \right) \vec{r} \]

\[ F_{pq} = F_{ij} = -\frac{3q}{r^5} \left[ 1 - \left( \frac{r}{r_c} \right)^2 \right] (\vec{p} \cdot \vec{r}) \vec{r} + \frac{q}{r^3} \left[ 1 - 3 \left( \frac{r}{r_c} \right)^2 + 2 \left( \frac{r}{r_c} \right)^3 \right] \vec{p} \]

\[ F_{qp} = F_{ij} = \frac{3q}{r^5} \left[ 1 - \left( \frac{r}{r_c} \right)^2 \right] (\vec{p} \cdot \vec{r}) \vec{r} - \frac{q}{r^3} \left[ 1 - 3 \left( \frac{r}{r_c} \right)^2 + 2 \left( \frac{r}{r_c} \right)^3 \right] \vec{p} \]

\[ F_{pp} = \frac{3}{r^5} \left\{ \left[ 1 - \left( \frac{r}{r_c} \right)^4 \right] \left[ (\vec{p}_i \cdot \vec{p}_j) - \frac{3}{r^2} (\vec{p}_i \cdot \vec{r})(\vec{p}_j \cdot \vec{r}) \right] \vec{r} + \right. \]
\[ \left. \left[ 1 - 4 \left( \frac{r}{r_c} \right)^3 + 3 \left( \frac{r}{r_c} \right)^4 \right] \left[ (\vec{p}_j \cdot \vec{r}) \vec{p}_i + (\vec{p}_i \cdot \vec{r}) \vec{p}_j - \frac{2}{r^2} (\vec{p}_i \cdot \vec{r})(\vec{p}_j \cdot \vec{r}) \vec{r} \right] \right\} \]
\[ T_{pq} = T_{ij} = \frac{q_i}{r^3} \left[ 1 - 3 \left( \frac{r}{r_c} \right)^2 + 2 \left( \frac{r}{r_c} \right)^3 \right] (\vec{p}_i \times \vec{r}) \]

\[ T_{qp} = T_{ji} = -\frac{q_i}{r^3} \left[ 1 - 3 \left( \frac{r}{r_c} \right)^2 + 2 \left( \frac{r}{r_c} \right)^3 \right] (\vec{p}_j \times \vec{r}) \]

\[ T_{pp} = T_{ij} = -\frac{1}{r^3} \left[ 1 - 4 \left( \frac{r}{r_c} \right)^3 + 6 \left( \frac{r}{r_c} \right)^4 \right] (\vec{p}_i \times \vec{p}_j) + \]

\[ \frac{3}{r^5} \left[ 1 - 4 \left( \frac{r}{r_c} \right)^3 + 3 \left( \frac{r}{r_c} \right)^4 \right] (\vec{p}_j \cdot \vec{r}) (\vec{p}_i \times \vec{r}) \]

\[ T_{pp} = T_{ji} = -\frac{1}{r^3} \left[ 1 - 4 \left( \frac{r}{r_c} \right)^3 + 3 \left( \frac{r}{r_c} \right)^4 \right] (\vec{p}_j \times \vec{p}_i) + \]

\[ \frac{3}{r^5} \left[ 1 - 4 \left( \frac{r}{r_c} \right)^3 + 3 \left( \frac{r}{r_c} \right)^4 \right] (\vec{p}_i \cdot \vec{r}) (\vec{p}_j \times \vec{r}) \]

where \( \epsilon \) and \( \sigma \) are the standard LJ parameters, \( r_c \) is the cutoff, \( q_i \) and \( q_j \) are the charges on the two particles, \( \vec{p}_i \) and \( \vec{p}_j \) are the dipole moment vectors of the two particles, \( r \) is their separation distance, and the vector \( \vec{r} = \vec{R}_i - \vec{R}_j \) is the separation vector between the two particles. Note that \( E_{qq} \) and \( F_{qq} \) are simply Coulombic energy and force, \( F_{ij} = -F_{ji} \) as symmetric forces, and \( T_{ij} \neq -T_{ji} \) since the torques do not act symmetrically. The shifted-force formula for the Lennard-Jones potential is reported in (Stoddard). The original (unshifted) formulas for the electrostatic potentials, forces and torques can be found in (Price). The shifted-force electrostatic potentials have been obtained by applying equation 5.13 of (Allen). The formulas for the corresponding forces and torques have been obtained by applying the 'chain rule' as in appendix C.3 of (Allen).

If one cutoff is specified in the pair_style command, it is used for both the LJ and Coulombic \((q,p)\) terms. If two cutoffs are specified, they are used as cutoffs for the LJ and Coulombic \((q,p)\) terms respectively.

Atoms with dipole moments should be integrated using the \texttt{fix nve/sphere update dipole} command to rotate the dipole moments. The \texttt{compute temp/sphere} command can be used to monitor the temperature, since it includes rotational degrees of freedom. The \texttt{atom_style dipole} command should be used since it defines the point dipoles and their rotational state. The magnitude of the dipole moment for each type of particle can be defined by the \texttt{dipole} command or in the "Dipoles" section of the data file read in by the \texttt{read_data} command. Their initial orientation can be defined by the \texttt{set dipole} command or in the "Atoms" section of the data file.

The following coefficients must be defined for each pair of atoms types via the \texttt{pair_coeff} command as in the examples above, or in the data file or restart files read by the \texttt{read_data} or \texttt{read_restart} commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff1 (distance units)
• cutoff2 (distance units)

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair.

Styles with a *cuda*, *gpu*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distances for this pair style can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

For atom type pairs I,J and I != J, the A, sigma, d1, and d2 coefficients and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. D1 and d2 are distance values and are mixed like sigma. The default mix value is geometric. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction; such energy goes to zero at the cutoff by construction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

**Restrictions:**

The dipole/cut style is part of the DIPOLE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The dipole/sf style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.
Related commands:
pair_coeff

Default: none


pair_style dpd command

pair_style dpd/omp command

pair_style dpd/tstat command

pair_style dpd/tstat/omp command

Syntax:

pair_style dpd T cutoff seed
pair_style dpd/tstat Tstart Tstop cutoff seed

• T = temperature (temperature units)
• Tstart, Tstop = desired temperature at start/end of run (temperature units)
• cutoff = global cutoff for DPD interactions (distance units)
• seed = random # seed (positive integer)

Examples:

pair_style dpd 1.0 2.5 34387
pair_coeff * * 3.0 1.0
pair_coeff 1 1 3.0 1.0 1.0

pair_style dpd/tstat 1.0 1.0 2.5 34387
pair_coeff * * 1.0
pair_coeff 1 1 1.0 1.0

Description:

Style dpd computes a force field for dissipative particle dynamics (DPD) following the exposition in (Groot).

Style dpd/tstat invokes a DPD thermostat on pairwise interactions, which is equivalent to the non-conservative portion of the DPD force field. This thermostat can be used in conjunction with any pair style, and in lieu of per-particle thermostats like fix langevin or ensemble thermostats like Nose Hoover as implemented by fix nvt. To use dpd/stat with another pair style, use the pair_style hybrid/overlay command to compute both the desired pair interaction and the thermostat for each pair of particles.

For style dpd, the force on atom I due to atom J is given as a sum of 3 terms
\[ \vec{f} = (F^C + F^D + F^R) \hat{r}_{ij} \quad r < r_c \]

\[ F^C = A w(r) \]

\[ F^D = -\gamma w^2(r) (\hat{r}_{ij} \cdot \vec{v}_{ij}) \]

\[ F^R = \sigma w(r) \alpha (\Delta t)^{-1/2} \]

\[ w(r) = 1 - r/r_c \]

where \( F_c \) is a conservative force, \( F_d \) is a dissipative force, and \( F_r \) is a random force. \( \hat{r}_{ij} \) is a unit vector in the direction \( \vec{R}_i - \vec{R}_j \), \( \vec{v}_{ij} \) is the vector difference in velocities of the two atoms = \( \vec{V}_i - \vec{V}_j \), \( \alpha \) is a Gaussian random number with zero mean and unit variance, \( \Delta t \) is the timestep size, and \( w(r) \) is a weighting factor that varies between 0 and 1. \( R_c \) is the cutoff. \( \sigma \) is set equal to \( \sqrt{2 K_b T \gamma} \), where \( K_b \) is the Boltzmann constant and \( T \) is the temperature parameter in the pair_style command.

For style \texttt{dpd/tstat}, the force on atom \( I \) due to atom \( J \) is the same as the above equation, except that the conservative \( F_c \) term is dropped. Also, during the run, \( T \) is set each timestep to a ramped value from \( T_{\text{start}} \) to \( T_{\text{stop}} \).

For style \texttt{dpd}, the pairwise energy associated with style \texttt{dpd} is only due to the conservative force term \( F_c \), and is shifted to be zero at the cutoff distance \( R_c \). The pairwise virial is calculated using all 3 terms. For style \texttt{dpd/tstat} there is no pairwise energy, but the last two terms of the formula make a contribution to the virial.

For style \texttt{dpd}, the following coefficients must be defined for each pair of atoms types via the \texttt{pair_coeff} command as in the examples above, or in the data file or restart files read by the \texttt{read_data} or \texttt{read_restart} commands:

- A (force units)
- gamma (force/velocity units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global DPD cutoff is used. Note that \( \sigma \) is set equal to \( \sqrt{2 T \gamma} \), where \( T \) is the temperature set by the \texttt{pair_style} command so it does not need to be specified.

For style \texttt{dpd/tstat}, the coefficients defined for each pair of atoms types via the \texttt{pair_coeff} command is the same, except that \( A \) is not included.

Styles with a \texttt{cuda}, \texttt{gpu}, \texttt{omp}, or \texttt{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \texttt{-suffix} command-line switch when you invoke LAMMPS, or you can use the \texttt{suffix} command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.
Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These pair styles do not support the pair_modify shift option for the energy of the pair interaction. Note that as discussed above, the energy due to the conservative Fc term is already shifted to be 0.0 at the cutoff distance Rc.

The pair_modify table option is not relevant for these pair styles.

These pair style do not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

These pair styles writes their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file. Note that the user-specified random number seed is stored in the restart file, so when a simulation is restarted, each processor will re-initialize its random number generator the same way it did initially. This means the random forces will be random, but will not be the same as they would have been if the original simulation had continued past the restart time.

These pair styles can only be used via the pair keyword of the run_style respa command. They do not support the inner, middle, outer keywords.

The dpd/tstat style can ramp its target temperature over multiple runs, using the start and stop keywords of the run command. See the run command for details of how to do this.

Restrictions:

The default frequency for rebuilding neighbor lists is every 10 steps (see the neigh_modify command). This may be too infrequent for style dpd simulations since particles move rapidly and can overlap by large amounts. If this setting yields a non-zero number of "dangerous" reneighborings (printed at the end of a simulation), you should experiment with forcing reneighboring more often and see if system energies/trajectories change.

These pair styles requires you to use the communicate vel yes option so that velocites are stored by ghost atoms.

These pair styles will not restart exactly when using the read_restart command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the read_restart command for more details.

Related commands:

pair_coeff, fix nvt, fix langevin

Default: none

pair_style dsmc command

Syntax:

pair_style dsmc max_cell_size seed weighting Tref Nrecompute Nsample

- max_cell_size = global maximum cell size for DSMC interactions (distance units)
- seed = random # seed (positive integer)
- weighting = macroparticle weighting
- Tref = reference temperature (temperature units)
- Nrecompute = recompute v*sigma_max every this many timesteps (timesteps)
- Nsample = sample this many times in recomputing v*sigma_max

Examples:

pair_style dsmc 2.5 34387 10 1.0 100 20
pair_coeff * * 1.0
pair_coeff 1 1 1.0

Description:

Style dsmc computes collisions between pairs of particles for a direct simulation Monte Carlo (DSMC) model following the exposition in (Bird). Each collision resets the velocities of the two particles involved. The number of pairwise collisions for each pair or particle types and the length scale within which they occur are determined by the parameters of the pair_style and pair_coeff commands.

Stochastic collisions are performed using the variable hard sphere (VHS) approach, with the user-defined max_cell_size value used as the maximum DSMC cell size, and reference cross-sections for collisions given using the pair_coeff command.

There is no pairwise energy or virial contributions associated with this pair style.

The following coefficient must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- sigma (area units, i.e. distance-squared)

The global DSMC max_cell_size determines the maximum cell length used in the DSMC calculation. A structured mesh is overlayed on the simulation box such that an integer number of cells are created in each direction for each processor's sub-domain. Cell lengths are adjusted up to the user-specifed maximum cell size.

To perform a DSMC simulation with LAMMPS, several additional options should be set in your input script, though LAMMPS does not check for these settings.

Since this pair style does not compute particle forces, you should use the "fix nve/noforce" time integration fix for the DSMC particles, e.g.

fix 1 all nve/noforce

This pair style assumes that all particles will communicated to neighboring processors every timestep as they move. This makes it possible to perform all collisions between pairs of particles that are on the same processor.
To ensure this occurs, you should use these commands:

```plaintext
neighbor 0.0 bin
neigh_modify every 1 delay 0 check no
communicate single cutoff 0.0
```

These commands insure that LAMMPS communicates particles to neighboring processors every timestep and that no ghost atoms are created. The output statistics for a simulation run should indicate there are no ghost particles or neighbors.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This pair style does not support the `pair_modify` shift option for the energy of the pair interaction.

The `pair_modify` table option is not relevant for this pair style.

This pair style does not support the `pair_modify` tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so `pair_style` and `pair_coeff` commands do not need to be specified in an input script that reads a restart file. Note that the user-specified random number seed is stored in the restart file, so when a simulation is restarted, each processor will re-initialize its random number generator the same way it did initially. This means the random forces will be random, but will not be the same as they would have been if the original simulation had continued past the restart time.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner, middle, outer` keywords.

**Restrictions:**

This style is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

`pair_coeff`, `fix nve/noforce`, `neigh_modify`, `neighbor`, `communicate`

**Default:** none

pair_style eam command
pair_style eam/cuda command
pair_style eam/gpu command
pair_style eam/omp command
pair_style eam/opt command
pair_style eam/alloy command
pair_style eam/alloy/cuda command
pair_style eam/alloy/gpu command
pair_style eam/alloy/omp command
pair_style eam/alloy/opt command
pair_style eam/cd command
pair_style eam/cd/omp command
pair_style eam/fs command
pair_style eam/fs/cuda command
pair_style eam/fs/gpu command
pair_style eam/fs/omp command
pair_style eam/fs/opt command

Syntax:

pair_style style

• style = eam or eam/alloy or eam/cd or eam/fs

Examples:

pair_style eam
pair_coeff * * cuu3
pair_coeff 1*3 1*3 niu3.eam

pair_style eam/alloy
Description:

Style *eam* computes pairwise interactions for metals and metal alloys using embedded-atom method (EAM) potentials (*Daw*). The total energy $E_i$ of an atom $I$ is given by

$$ E_i = F_\alpha \left( \sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij}) $$

where $F$ is the embedding energy which is a function of the atomic electron density $\rho$, $\phi$ is a pair potential interaction, and $\alpha$ and $\beta$ are the element types of atoms $I$ and $J$. The multi-body nature of the EAM potential is a result of the embedding energy term. Both summations in the formula are over all neighbors $J$ of atom $I$ within the cutoff distance.

The cutoff distance and the tabulated values of the functionals $F$, $\rho$, and $\phi$ are listed in one or more files which are specified by the *pair_coeff* command. These are ASCII text files in a DYNAMO-style format which is described below. DYNAMO was the original serial EAM MD code, written by the EAM originators. Several DYNAMO potential files for different metals are included in the "potentials" directory of the LAMMPS distribution. All of these files are parameterized in terms of LAMMPS metal units.

**IMPORTANT NOTE:** The *eam* style reads single-element EAM potentials in the DYNAMO *funcfl* format. Either single element or alloy systems can be modeled using multiple *funcfl* files and style *eam*. For the alloy case LAMMPS mixes the single-element potentials to produce alloy potentials, the same way that DYNAMO does. Alternatively, a single DYNAMO *setfl* file or Finnis/Sinclair EAM file can be used by LAMMPS to model alloy systems by invoking the *eam/alloy* or *eam/cd* or *eam/fs* styles as described below. These files require no mixing since they specify alloy interactions explicitly.

Note that unlike for other potentials, cutoffs for EAM potentials are not set in the *pair_style* or *pair_coeff* command; they are specified in the EAM potential files themselves. Likewise, the EAM potential files list atomic masses; thus you do not need to use the *mass* command to specify them.

There are several WWW sites that distribute and document EAM potentials stored in DYNAMO or other formats:

- [http://www.ctcms.nist.gov/potentials](http://www.ctcms.nist.gov/potentials)

These potentials should be usable with LAMMPS, though the alternate formats would need to be converted to the DYNAMO format used by LAMMPS and described on this page. The NIST site is maintained by Chandler Becker (cbecker at nist.gov) who is good resource for info on interatomic potentials and file formats.

For style *eam*, potential values are read from a file that is in the DYNAMO single-element *funcfl* format. If the
DYNAMO file was created by a Fortran program, it cannot have "D" values in it for exponents. C only recognizes "e" or "E" for scientific notation.

Note that unlike for other potentials, cutoffs for EAM potentials are not set in the pair_style or pair_coeff command; they are specified in the EAM potential files themselves.

For style *eam* a potential file must be assigned to each I,I pair of atom types by using one or more pair_coeff commands, each with a single argument:

- `filename`

Thus the following command

```
pair_coeff *2 1*2 cuu3.eam
```

will read the cuu3 potential file and use the tabulated Cu values for F, phi, rho that it contains for type pairs 1,1 and 2,2 (type pairs 1,2 and 2,1 are ignored). In effect, this makes atom types 1 and 2 in LAMMPS be Cu atoms. Different single-element files can be assigned to different atom types to model an alloy system. The mixing to create alloy potentials for type pairs with I != J is done automatically the same way that the serial DYNAMO code originally did it; you do not need to specify coefficients for these type pairs.

*funcfl* files in the *potentials* directory of the LAMMPS distribution have an ".eam" suffix. A DYNAMO single-element *funcfl* file is formatted as follows:

- line 1: comment (ignored)
- line 2: atomic number, mass, lattice constant, lattice type (e.g. FCC)
- line 3: Nrho, drho, Nr, dr, cutoff

On line 2, all values but the mass are ignored by LAMMPS. The mass is in mass units, e.g. mass number or grams/mole for metal units. The cubic lattice constant is in Angstroms. On line 3, Nrho and Nr are the number of tabulated values in the subsequent arrays, drho and dr are the spacing in density and distance space for the values in those arrays, and the specified cutoff becomes the pairwise cutoff used by LAMMPS for the potential. The units of dr are Angstroms; I'm not sure of the units for drho - some measure of electron density.

Following the three header lines are three arrays of tabulated values:

- embedding function F(rho) (Nrho values)
- effective charge function Z(r) (Nr values)
- density function rho(r) (Nr values)

The values for each array can be listed as multiple values per line, so long as each array starts on a new line. For example, the individual Z(r) values are for r = 0,dr,2*dr, ... (Nr-1)*dr.

The units for the embedding function F are eV. The units for the density function rho are the same as for drho (see above, electron density). The units for the effective charge Z are "atomic charge" or sqrt(Hartree * Bohr-radii). For two interacting atoms i,j this is used by LAMMPS to compute the pair potential term in the EAM energy expression as r*phi, in units of eV-Angstroms, via the formula

```
r*phi = 27.2 * 0.529 * Zi * Zj
```

where 1 Hartree = 27.2 eV and 1 Bohr = 0.529 Angstroms.
Style *eam/alloy* computes pairwise interactions using the same formula as style *eam*. However the associated *pair_coeff* command reads a DYNAMO *setfl* file instead of a *funcfl* file. *Setfl* files can be used to model a single-element or alloy system. In the alloy case, as explained above, *setfl* files contain explicit tabulated values for alloy interactions. Thus they allow more generality than *funcfl* files for modeling alloys.

For style *eam/alloy*, potential values are read from a file that is in the DYNAMO multi-element *setfl* format, except that element names (Ni, Cu, etc) are added to one of the lines in the file. If the DYNAMO file was created by a Fortran program, it cannot have "D" values in it for exponents. C only recognizes "e" or "E" for scientific notation.

Only a single *pair_coeff* command is used with the *eam/alloy* style which specifies a DYNAMO *setfl* file, which contains information for M elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the *pair_coeff* command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of *setfl* elements to atom types

As an example, the potentials/NiAlH_jea.eam.alloy file is a *setfl* file which has tabulated EAM values for 3 elements and their alloy interactions: Ni, Al, and H. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Ni, and the 4th to be Al, you would use the following *pair_coeff* command:

```
pair_coeff * * NiAlH_jea.eam.alloy Ni Ni Ni Al
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Ni arguments map LAMMPS atom types 1,2,3 to the Ni element in the *setfl* file. The final Al argument maps LAMMPS atom type 4 to the Al element in the *setfl* file. Note that there is no requirement that your simulation use all the elements specified by the *setfl* file.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when an *eam/alloy* potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

*Setfl* files in the *potentials* directory of the LAMMPS distribution have an ".eam.alloy" suffix. A DYNAMO multi-element *setfl* file is formatted as follows:

- lines 1,2,3 = comments (ignored)
- line 4: Nelements Element1 Element2 ... ElementN
- line 5: Nrho, drho, Nr, dr, cutoff

In a DYNAMO *setfl* file, line 4 only lists Nelements = the # of elements in the *setfl* file. For LAMMPS, the element name (Ni, Cu, etc) of each element must be added to the line, in the order the elements appear in the file.

The meaning and units of the values in line 5 is the same as for the *funcfl* file described above. Note that the cutoff (in Angstroms) is a global value, valid for all pairwise interactions for all element pairings.

Following the 5 header lines are Nelements sections, one for each element, each with the following format:

- line 1 = atomic number, mass, lattice constant, lattice type (e.g. FCC)
- embedding function F(rho) (Nrho values)
- density function rho(r) (Nr values)

As with the *funcfl* files, only the mass (in mass units, e.g. mass number or grams/mole for metal units) is used by LAMMPS from the 1st line. The cubic lattice constant is in Angstroms. The F and rho arrays are unique to a
single element and have the same format and units as in a `funcfl` file.

Following the Nelements sections, Nr values for each pair potential phi(r) array are listed for all i,j element pairs in the same format as other arrays. Since these interactions are symmetric (i,j = j,i) only phi arrays with i >= j are listed, in the following order: i,j = (1,1), (2,1), (2,2), (3,1), (3,2), (3,3), (4,1), ..., (Nelements, Nelements). Unlike the effective charge array Z(r) in `funcfl` files, the tabulated values for each phi function are listed in `setfl` files directly as r*phi (in units of eV-Angstroms), since they are for atom pairs.

Style `eam/cd` is similar to the `eam/alloy` style, except that it computes alloy pairwise interactions using the concentration-dependent embedded-atom method (CD-EAM). This model can reproduce the enthalpy of mixing of alloys over the full composition range, as described in (Stukowski).

The pair_coeff command is specified the same as for the `eam/alloy` style. However the DYNAMO `setfl` file must has two lines added to it, at the end of the file:

- line 1: Comment line (ignored)
- line 2: N Coefficient0 Coefficient1 ... CoeffincientN

The last line begins with the degree N of the polynomial function h(x) that modifies the cross interaction between A and B elements. Then N+1 coefficients for the terms of the polynomial are then listed.

Modified EAM `setfl` files used with the `eam/cd` style must contain exactly two elements, i.e. in the current implementation the `eam/cd` style only supports binary alloys. The first and second elements in the input EAM file are always taken as the A and B species.

`CD-EAM` files in the `potentials` directory of the LAMMPS distribution have a ".cdeam" suffix.

Style `eam/fs` computes pairwise interactions for metals and metal alloys using a generalized form of EAM potentials due to Finnis and Sinclair (Finnis). The total energy Ei of an atom I is given by

$$E_i = F_\alpha \left( \sum_{j \neq i} \rho_{\alpha\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

This has the same form as the EAM formula above, except that rho is now a functional specific to the atomic types of both atoms I and J, so that different elements can contribute differently to the total electron density at an atomic site depending on the identity of the element at that atomic site.

The associated pair_coeff command for style `eam/fs` reads a DYNAMO `setfl` file that has been extended to include additional rho_alpha_beta arrays of tabulated values. A discussion of how FS EAM differs from conventional EAM alloy potentials is given in (Ackland1). An example of such a potential is the same author's Fe-P FS potential (Ackland2). Note that while FS potentials always specify the embedding energy with a square root dependence on the total density, the implementation in LAMMPS does not require that; the user can tabulate any functional form desired in the FS potential files.

For style `eam/fs`, the form of the pair_coeff command is exactly the same as for style `eam/alloy`, e.g.

```
pair_coeff * * NiAlH_jea.eam.fs Ni Ni Ni Al
```
where there are N additional arguments after the filename, where N is the number of LAMMPS atom types. The N values determine the mapping of LAMMPS atom types to EAM elements in the file, as described above for style eam/alloy. As with eam/alloy, if a mapping value is NULL, the mapping is not performed. This can be used when an eam/fs potential is used as part of the hybrid pair style. The NULL values are used as placeholders for atom types that will be used with other potentials.

FS EAM files include more information than the DYNAMO setfl format files read by eam/alloy, in that i,j density functionals for all pairs of elements are included as needed by the Finnis/Sinclair formulation of the EAM.

FS EAM files in the potentials directory of the LAMMPS distribution have an ".eam.fs" suffix. They are formatted as follows:

- lines 1,2,3 = comments (ignored)
- line 4: Nelements Element1 Element2 ... ElementN
- line 5: Nrho, drho, Nr, dr, cutoff

The 5-line header section is identical to an EAM setfl file.

Following the header are Nelements sections, one for each element I, each with the following format:

- line 1 = atomic number, mass, lattice constant, lattice type (e.g. FCC)
- embedding function F(rho) (Nrho values)
- density function rho(r) for element I at element 1 (Nr values)
- density function rho(r) for element I at element 2
- ...
- density function rho(r) for element I at element Nelement

The units of these quantities in line 1 are the same as for setfl files. Note that the rho(r) arrays in Finnis/Sinclair can be asymmetric (i,j != j,i) so there are Nelements^2 of them listed in the file.

Following the Nelements sections, Nr values for each pair potential phi(r) array are listed in the same manner (r*phi, units of eV-Angstroms) as in EAM setfl files. Note that in Finnis/Sinclair, the phi(r) arrays are still symmetric, so only phi arrays for i >= j are listed.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelearate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelearate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs IJ and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above with the individual styles. You never need to specify a pair_coeff
command with $I \neq J$ arguments for the eam styles.

This pair style does not support the `pair_modify` shift, table, and tail options.

The eam pair styles do not write their information to binary restart files, since it is stored in tabulated potential files. Thus, you need to re-specify the `pair_style` and `pair_coeff` commands in an input script that reads a restart file.

The eam pair styles can only be used via the `pair` keyword of the `run_style respa` command. They do not support the `inner`, `middle`, `outer` keywords.

**Restrictions:**

All of these styles except the eam/cd style are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

The eam/cd style is part of the USER-MISC package and also requires the MANYBODY package. It is only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

**Related commands:**

`pair_coeff`

**Default:** none


(Stukowski) Stukowski, Sadigh, Erhart, Caro; Modeling Simulation Materials Science & Engineering, 7, 075005 (2009).
pair_style edip command

Syntax:

pair_style edip

Examples:

pair_style edip pair_coeff ** Si.edip Si

Description:

The edip style computes a 3-body EDIP potential which is popular for modeling silicon materials where it can have advantages over other models such as the Stillinger-Weber or Tersoff potentials. In EDIP, the energy $E$ of a system of atoms is

$$E = \sum_{j \neq i} \phi_2(R_{ij}, Z_i) + \sum_{j \neq i} \sum_{k \neq i, k > j} \phi_3(R_{ij}, R_{ik}, Z_i)$$

$$\phi_2(r, Z) = A \left[ \left( \frac{B}{r} \right)^{\rho} - e^{-\beta Z^2} \right] \exp \left( \frac{\sigma}{r - a} \right)$$

$$\phi_3(R_{ij}, R_{ik}, Z_i) = \exp \left( \frac{\gamma}{R_{ij} - a} \right) \exp \left( \frac{\gamma}{R_{ik} - a} \right) h(\cos\theta_{ijk}, Z_i)$$

$$Z_i = \sum_{m \neq i} f(R_{im})$$

$$f(r) = \begin{cases} 
1 & r < c \\
\exp \left( \frac{\alpha}{1-x^{-3}} \right) & c < r < a \\
0 & r > a 
\end{cases}$$

$$h(l, Z) = \lambda [(1 - e^{-Q(Z)(l+\tau(Z))^2}) + \eta Q(Z)(l + \tau(Z))^2]$$

$$Q(Z) = Q_0 e^{-\mu Z}$$

$$\tau(Z) = u_1 + u_2 (u_3 e^{-u_4 Z} - e^{-2u_4 Z})$$

where $\phi_2$ is a two-body term and $\phi_3$ is a three-body term. The summations in the formula are over all neighbors $J$ and $K$ of atom $I$ within a cutoff distance $= a$. Both terms depend on the local environment of atom $I$ through its effective coordination number defined by $Z$, which is unity for a cutoff distance $< c$ and gently goes to 0 at distance $= a$.

Only a single pair_coeff command is used with the edip style which specifies a EDIP potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying $N$ additional
arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of EDIP elements to atom types

As an example, imagine a file Si.edip has EDIP values for Si.

EDIP files in the potentials directory of the LAMMPS distribution have a ".edip" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to the two-body and three-body coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2
- element 3
- A (energy units)
- B (distance units)
- cutoffA (distance units)
- cutoffC (distance units)
- alpha
- beta
- eta
- gamma (distance units)
- lambda (energy units)
- mu
- tho
- sigma (distance units)
- Q0
- u1
- u2
- u3
- u4

The A, B, beta, sigma parameters are used only for two-body interactions. The eta, gamma, lambda, mu, Q0 and all u1 to u4 parameters are used only for three-body interactions. The alpha and cutoffC parameters are used for the coordination environment function only.

The EDIP potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify EDIP parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

At the moment, only a single element parametrization is implemented. However, the author is not aware of other multi-element EDIP parametrizations. If you know any and you are interest in that, please contact the author of the EDIP package.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.
These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

This pair style requires the newton setting to be "on" for pair interactions.

The EDIP potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the SW potential with any LAMMPS units, but you would need to create your own EDIP potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none

pair_style eff/cut command

Syntax:

pair_style eff/cut cutoff eradius_limit_flag pressure_flag

- cutoff = global cutoff for Coulombic interactions
- eradius_limit_flag = 0 or 1 for whether electron size is restrained (optional)
- pressure_flag = 0 or 1 to define the type of pressure calculation (optional)

Examples:

```
pair_style eff/cut 39.7
pair_style eff/cut 40.0 1 1
pair_coeff * *
pair_coeff 2 2 20.0
```

Description:

This pair style contains a LAMMPS implementation of the electron Force Field (eFF) potential currently under development at Caltech, as described in [Jaramillo-Botero]. The eFF was first introduced by [Su] in 2007.

eFF can be viewed as an approximation to QM wave packet dynamics and Fermionic molecular dynamics, combining the ability of electronic structure methods to describe atomic structure, bonding, and chemistry in materials, and of plasma methods to describe nonequilibrium dynamics of large systems with a large number of highly excited electrons. Yet, eFF relies on a simplification of the electronic wavefunction in which electrons are described as floating Gaussian wave packets whose position and size respond to the various dynamic forces between interacting classical nuclear particles and spherical Gaussian electron wavepackets. The wavefunction is taken to be a Hartree product of the wave packets. To compensate for the lack of explicit antisymmetry in the resulting wavefunction, a spin-dependent Pauli potential is included in the Hamiltonian. Substituting this wavefunction into the time-dependent Schrödinger equation produces equations of motion that correspond - to second order - to classical Hamiltonian relations between electron position and size, and their conjugate momenta. The N-electron wavefunction is described as a product of one-electron Gaussian functions, whose size is a dynamical variable and whose position is not constrained to a nuclear center. This form allows for straightforward propagation of the wavefunction, with time, using a simple formulation from which the equations of motion are then integrated with conventional MD algorithms. In addition to this spin-dependent Pauli repulsion potential term between Gaussians, eFF includes the electron kinetic energy from the Gaussians. These two terms are based on first-principles quantum mechanics. On the other hand, nuclei are described as point charges, which interact with other nuclei and electrons through standard electrostatic potential forms.

The full Hamiltonian (shown below), contains then a standard description for electrostatic interactions between a set of delocalized point and Gaussian charges which include, nuclei-nuclei (NN), electron-electron (ee), and nuclei-electron (Ne). Thus, eFF is a mixed QM-classical mechanics method rather than a conventional force field method (in which electron motions are averaged out into ground state nuclear motions, i.e a single electronic state, and particle interactions are described via empirically parameterized interatomic potential functions). This makes eFF uniquely suited to simulate materials over a wide range of temperatures and pressures where electronically excited and ionized states of matter can occur and coexist. Furthermore, the interactions between particles -nuclei and electrons- reduce to the sum of a set of effective pairwise potentials in the eFF formulation. The eff/cut style computes the pairwise Coulomb interactions between nuclei and electrons ($E_{\text{NN}}, E_{\text{Ne}}, E_{\text{ee}}$), and the quantum-derived Pauli ($E_{\text{PR}}$) and Kinetic energy interactions potentials between electrons ($E_{\text{KE}}$) for a total energy expression given as,
\[ U(R, r, s) = E_{NN}(R) + E_{Ne}(R, r, s) + E_{ee}(r, s) + E_{KE}(r, s) + E_{PR}(\uparrow \downarrow, S) \]

The individual terms are defined as follows:

\[ E_{KE} = \frac{\hbar^2}{m_e} \sum_i \frac{3}{2s_i^2} \]

\[ E_{NN} = \frac{1}{4\pi\varepsilon_0} \sum_{i<j} \frac{Z_i Z_j}{R_{ij}} \]

\[ E_{Ne} = -\frac{1}{4\pi\varepsilon_0} \sum_{i,j} \frac{Z_i}{R_{ij}} E_{R} f \left( \frac{\sqrt{2}R_{ij}}{s_j} \right) \]

\[ E_{ee} = \frac{1}{4\pi\varepsilon_0} \sum_{i<j} \frac{1}{r_{ij}} E_{R} f \left( \frac{\sqrt{2}r_{ij}}{\sqrt{s_i^2 + s_j^2}} \right) \]

\[ E_{Pauli} = \sum_{\sigma_i=\sigma_j} E(\uparrow\uparrow)_{ij} + \sum_{\sigma_i\neq\sigma_j} E(\uparrow\downarrow)_{ij} \]

where, \( s_i \) correspond to the electron sizes, the sigmas i's to the fixed spins of the electrons, \( Z_i \) to the charges on the nuclei, \( R_{ij} \) to the distances between the nuclei or the nuclei and electrons, and \( r_{ij} \) to the distances between electrons. For additional details see (Jaramillo-Botero).

The overall electrostatics energy is given in Hartree units of energy by default and can be modified by an energy-conversion constant, according to the units chosen (see electron_units). The cutoff \( R_c \), given in Bohrs (by default), truncates the interaction distance. The recommended cutoff for this pair style should follow the minimum image criterion, i.e. half of the minimum unit cell length.

Style \textit{eff/long} (not yet available) computes the same interactions as style \textit{eff/cut} except that an additional damping factor is applied so it can be used in conjunction with the \textit{kspace_style} command and its \textit{ewald} or \textit{pppm} option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed.
directly; interactions outside that distance are computed in reciprocal space.

This potential is designed to be used with atom_style electron definitions, in order to handle the description of systems with interacting nuclei and explicit electrons.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- cutoff (distance units)

For eff/cut, the cutoff coefficient is optional. If it is not used (as in some of the examples above), the default global value specified in the pair_style command is used.

For eff/long (not yet available) no cutoff will be specified for an individual I,J type pair via the pair_coeff command. All type pairs use the same global cutoff specified in the pair_style command.

The eradius_limit_flag and pressure_flag settings are optional. Neither or both must be specified. If not specified they are both set to 0 by default.

The eradius_limit_flag is used to restrain electrons from becoming unbounded in size at very high temperatures were the Gaussian wave packet representation breaks down, and from expanding as free particles to infinite size. A setting of 0 means do not impose this restraint. A setting of 1 imposes the restraint. The restraining harmonic potential takes the form E = 1/2k_s s^2 for s > L_box/2, where k_s = 1 Hartrees/Bohr^2.

The pressure_flag is used to control between two types of pressure computation: if set to 0, the computed pressure does not include the electronic radial virials contributions to the total pressure (scalar or tensor). If set to 1, the computed pressure will include the electronic radial virial contributions to the total pressure (scalar and tensor).

IMPORTANT NOTE: there are two different pressures that can be reported for eFF when defining this pair_style, one (default) that considers electrons do not contribute radial virial components (i.e. electrons treated as incompressible 'rigid' spheres) and one that does. The radial electronic contributions to the virials are only tallied if the flexible pressure option is set, and this will affect both global and per-atom quantities. In principle, the true pressure of a system is somewhere in between the rigid and the flexible eFF pressures, but, for most cases, the difference between these two pressures will not be significant over long-term averaged runs (i.e. even though the energy partitioning changes, the total energy remains similar).

IMPORTANT NOTE: The currently implemented eFF gives a reasonably accurate description for systems containing nuclei from Z = 1-6. Users interested in applying eFF should restrict to systems where electrons are s-like, or contain p character only insofar as a single lobe of electron density is shifted away from the nuclear center. See further details about some of the virtues and current limitations of the method in (Jaramillo-Botero).

Work is underway to extend the eFF to higher Z elements with increasingly non-spherical electrons (p-block and d-block), to provide explicit terms for electron correlation/exchange, and to improve its computational efficiency via atom models with fixed 2 s core electrons and atom models represented as pseudo-cores plus valence electrons.

The current version adds support for models with fixed-core and effective pseudo-core (i.e. effective core pseudopotentials, ECP) definitions. to enable larger timesteps (i.e. by avoiding the high frequency vibrational modes -translational and radial- of the 2 s electrons), and in the ECP case to reduce the p-character effects in higher Z elements (e.g. Silicon). A fixed-core should be defined with a mass that includes the corresponding nuclear mass plus the 2 s electrons in atomic mass units (2x5.4857990943e-4), and a radius equivalent to that of...
minimized 1s electrons (see examples under /examples/USER/eff/fixed-core). An pseudo-core should be described with a mass that includes the corresponding nuclear mass, plus all the core electrons (i.e. no outer shell electrons), and a radius equivalent to that of a corresponding minimized full-electron system. The charge for a pseudo-core atom should be given by the number of outer shell electrons.

In general, eFF excels at computing the properties of materials in extreme conditions and tracing the system dynamics over multi-picosecond timescales; this is particularly relevant where electron excitations can change significantly the nature of bonding in the system. It can capture with surprising accuracy the behavior of such systems because it describes consistently and in an unbiased manner many different kinds of bonds, including covalent, ionic, multicenter, ionic, and plasma, and how they interconvert and/or change when they become excited. eFF also excels in computing the relative thermochemistry of isodemic reactions and conformational changes, where the bonds of the reactants are of the same type as the bonds of the products. eFF assumes that kinetic energy differences dominate the overall exchange energy, which is true when the electrons present are nearly spherical and nodeless and valid for covalent compounds such as dense hydrogen, hydrocarbons, and diamond; alkali metals (e.g. lithium), alkali earth metals (e.g. beryllium) and semimetals such as boron; and various compounds containing ionic and/or multicenter bonds, such as boron dihydride.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the cutoff distance for the eff/cut style can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

The pair_modify shift option is not relevant for these pair styles.

The eff/long (not yet available) style supports the pair_modify table option for tabulation of the short-range portion of the long-range Coulombic interaction.

These pair styles do not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

These pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the pair keyword of the run_style respa command. They do not support the inner, middle, outer keywords.

Restrictions:

These pair styles will only be enabled if LAMMPS is built with the USER-EFF package. It will only be enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

These pair styles require that particles store electron attributes such as radius, radial velocity, and radial force, as defined by the atom_style. The electron atom style does all of this.

These pair styles require you to use the communicate vel yes option so that velocities are stored by ghost atoms.

Related commands:

pair_coeff

Default:
If not specified, eradius_limit_flag = 0 and pressure_flag = 0.


**pair_style eim command**

**pair_style eim/omp command**

**Syntax:**

```
pair_style style
  • style = eim
```

**Examples:**

```
pair_style eim
pair_coeff * * Na Cl ../potentials/ffield.eim Na Cl
pair_coeff * * Na Cl ffield.eim Na Na Na Cl
pair_coeff * * Na Cl ../potentials/ffield.eim Cl NULL Na
```

**Description:**

Style *eim* computes pairwise interactions for ionic compounds using embedded-ion method (EIM) potentials (Zhou). The energy of the system $E$ is given by

$$
E = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=i_1}^{i_N} \phi_{ij} (r_{ij}) + \sum_{i=1}^{N} E_i (q_i, \sigma_i)
$$

The first term is a double pairwise sum over the J neighbors of all I atoms, where $\phi_{ij}$ is a pair potential. The second term sums over the embedding energy $E_i$ of atom I, which is a function of its charge $q_i$ and the electrical potential $\sigma_i$ at its location. $E_i$, $q_i$, and $\sigma_i$ are calculated as

$$
q_i = \sum_{j=i_1}^{i_N} \eta_{ji} (r_{ij})
$$

$$
\sigma_i = \sum_{j=i_1}^{i_N} q_j \cdot \psi_{ij} (r_{ij})
$$

$$
E_i (q_i, \sigma_i) = \frac{1}{2} \cdot q_i \cdot \sigma_i
$$

where $\eta_{ji}$ is a pairwise function describing electron flow from atom I to atom J, and $\psi_{ij}$ is another pairwise function. The multi-body nature of the EIM potential is a result of the embedding energy term. A complete list of all the pair functions used in EIM is summarized below.
\[
\begin{align*}
\langle r \rangle &= \left\{ \left[ \frac{E_{b,ij} \beta_{ij}}{\beta_{ij} - \alpha_{ij}} \right] \exp \left( \frac{-\alpha_{ij} - \frac{r - r_{e,ij}}{r_{e,ij}}}{\beta_{ij} - \alpha_{ij}} \right) - \frac{E_{b,ij} \alpha_{ij}}{\beta_{ij} - \alpha_{ij}} \right] \exp \left( \frac{-\beta_{ij} - \frac{r - r_{e,ij}}{r_{e,ij}}}{\beta_{ij} - \alpha_{ij}} \right) \right) f_c \left( r, r_{e,ij}, r_{c,\phi,ij} \right), \\
\eta_{ji} &= A_{\eta,ij} \left( \chi_j - \chi_i \right) f_c \left( r, r_{s,\eta,ij}, r_{c,\eta,ij} \right), \\
\psi_{ij} (r) &= A_{\psi,ij} \exp \left( -\zeta_{ij} r \right) f_c \left( r, r_{s,\psi,ij}, r_{c,\psi,ij} \right) \\
f_c \left( r, r_p, r_c \right) &= 0.510204erf \left[ \frac{1.64498 \left( 2r - r_p - r_c \right)}{r_c - r_p} \right] - 0.010204
\end{align*}
\]

Here \(E_{\text{b}}, r_{\text{e}}, r_{\text{(c,phi)}}, \alpha, \beta, A_{\text{(psi)}}, \zeta, r_{\text{(s,psi)}}, r_{\text{(c,psi)}}, A_{\text{(eta)}}, r_{\text{(s,eta)}}, r_{\text{(c,eta)}}, \chi, \) and pair function type \(p\) are parameters, with subscripts \(ij\) indicating the two species of atoms in the atomic pair.

**IMPORTANT NOTE:** Even though the EIM potential is treating atoms as charged ions, you should not use a LAMMPS atom_style that stores a charge on each atom and thus requires you to assign a charge to each atom, e.g. the charge or full atom styles. This is because the EIM potential infers the charge on an atom from the equation above for \(q_i\); you do not assign charges explicitly.

All the EIM parameters are listed in a potential file which is specified by the pair_coeff command. This is an ASCII text file in a format described below. The "ffield.eim" file included in the "potentials" directory of the LAMMPS distribution currently includes nine elements Li, Na, K, Rb, Cs, F, Cl, Br, and I. A system with any combination of these elements can be modeled. This file is parameterized in terms of LAMMPS metal units.

Note that unlike other potentials, cutoffs for EIM potentials are not set in the pair_style or pair_coeff command; they are specified in the EIM potential file itself. Likewise, the EIM potential file lists atomic masses; thus you do not need to use the mass command to specify them.

Only a single pair_coeff command is used with the eim style which specifies an EIM potential file and the element(s) to extract information for. The EIM elements are mapped to LAMMPS atom types by specifying \(N\) additional arguments after the filename in the pair_coeff command, where \(N\) is the number of LAMMPS atom types:

- Elem1, Elem2, ...
- EIM potential file
- \(N\) element names = mapping of EIM elements to atom types

As an example like one of those above, suppose you want to model a system with Na and Cl atoms. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Na, and the 4th to be Cl, you would use the
following pair_coeff command:

    pair_coeff * * Na Cl ffield.eim Na Na Na Cl

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The filename is the EIM potential file. The Na and Cl arguments (before the file name) are the two elements for which info will be extracted from the potential file. The first three trailing Na arguments map LAMMPS atom types 1,2,3 to the EIM Na element. The final Cl argument maps LAMMPS atom type 4 to the EIM Cl element.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when an eim potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The ffield.eim file in the potentials directory of the LAMMPS distribution is formatted as follows:

Lines starting with # are comments and are ignored by LAMMPS. Lines starting with "global:" include three global values. The first value divides the cations from anions, i.e., any elements with electronegativity above this value are viewed as anions, and any elements with electronegativity below this value are viewed as cations. The second and third values are related to the cutoff function - i.e. the 0.510204, 1.64498, and 0.010204 shown in the above equation can be derived from these values.

Lines starting with "element:" are formatted as follows: name of element, atomic number, atomic mass, electronic negativity, atomic radius (LAMMPS ignores it), ionic radius (LAMMPS ignores it), cohesive energy (LAMMPS ignores it), and q0 (must be 0).

Lines starting with "pair:" are entered as: element 1, element 2, r_(c,phi), r_(c,phi) (redundant for historical reasons), E_b, r_e, alpha, beta, r_(c,eta), A_(eta), r_(s,eta), r_(c,psi), A_(psi), zeta, r_(s,psi), and p.

The lines in the file can be in any order; LAMMPS extracts the info it needs.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default).

Related commands:

pair_coeff
(Zhou) Zhou, submitted for publication (2010). Please contact Xiaowang Zhou (Sandia) for details via email at xzhou at sandia.gov.
pair_style gauss command

pair_style gauss/gpu command

pair_style gauss/omp command

pair_style gauss/cut command

pair_style gauss/cut/omp command

Syntax:

pair_style gauss cutoff
pair_style gauss/cut cutoff

- cutoff = global cutoff for Gauss interactions (distance units)

Examples:

pair_style gauss 12.0
pair_coeff * * 1.0 0.9
pair_coeff 1 4 1.0 0.9 10.0

pair_style gauss/cut 3.5
pair_coeff 1 4 0.2805 1.45 0.112

Description:

Style gauss computes a tethering potential of the form

\[ E = A \exp(-Br^2) \quad r < r_c \]

between an atom and its corresponding tether site which will typically be a frozen atom in the simulation. Rc is the cutoff.

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A (energy units)
- B (1/distance^2 units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

Style gauss/cut computes a generalized Gaussian interaction potential between pairs of particles:
\[ E = \frac{H}{\sigma_h \sqrt{2\pi}} \exp \left[ -\frac{(r-r_{mh})^2}{2\sigma_h^2} \right] \]

where H determines together with the standard deviation sigma_h the peak height of the Gaussian function, and r_mh the peak position. Examples of the use of the Gaussian potentials include implicit solvent simulations of salt ions (Lenart) and of surfactants (Jusufi). In these instances the Gaussian potential mimics the hydration barrier between a pair of particles. The hydration barrier is located at r_mh and has a width of sigma_h. The prefactor determines the height of the potential barrier.

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- H (energy * distance units)
- r_mh (distance units)
- sigma_h (distance units)

The global cutoff (r_c) specified in the pair_style command is used.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the "-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair style do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The gauss style does not support the pair_modify shift option. There is no effect due to the Gaussian well beyond the cutoff; hence reasonable cutoffs need to be specified.

The gauss/cut style supports the pair_modify shift option for the energy of the Gauss-potential portion of the pair interaction.

The pair_modify table and tail options are not relevant for this pair style.

This pair style does not support the pair_modify table option, since a tabulation capability does not exist for this potential.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.
This pair style can only be used via the \textit{pair} keyword of the \texttt{run_style respa} command. It does not support the \textit{inner, middle, outer} keywords.

The \textit{gauss} pair style tallies an "occupancy" count of how many Gaussian-well sites have an atom within the distance at which the force is a maximum = \( \sqrt{0.5/b} \). This quantity can be accessed via the \texttt{compute pair} command as a vector of values of length 1.

To print this quantity to the log file (with a descriptive column heading) the following commands could be included in an input script:

\begin{verbatim}
compute gauss all pair gauss
variable occ equal c_gauss[1]
thermo_style custom step temp epair v_occ
\end{verbatim}

\textbf{Restrictions:}

The \textit{gauss/cut} style is part of the "user-misc" package. It is only enabled if LAMMPS is build with that package. See the \texttt{Making of LAMMPS} section for more info.

\textbf{Related commands:}

\texttt{pair_coeff}, \texttt{pair_style coul/diel}

\textbf{Default:} none
pair_style gayberne command

pair_style gayberne/gpu command

pair_style gayberne/omp command

Syntax:

pair_style gayberne gamma upsilon mu cutoff

- gamma = shift for potential minimum (typically 1)
- upsilon = exponent for eta orientation-dependent energy function
- mu = exponent for chi orientation-dependent energy function
- cutoff = global cutoff for interactions (distance units)

Examples:

pair_style gayberne 1.0 1.0 1.0 10.0
pair_coeff * * 1.0 1.7 1.7 3.4 3.4 1.0 1.0 1.0

Description:

The gayberne styles compute a Gay-Berne anisotropic LJ interaction (Berardi) between pairs of ellipsoidal particles or an ellipsoidal and spherical particle via the formulas

\[
U(A_1, A_2, r_{12}) = U_r(A_1, A_2, r_{12}, \gamma) \cdot \eta_{12}(A_1, A_2, \upsilon) \cdot \chi_{12}(A_1, A_2, r_{12}, \mu)
\]

\[
U_r = 4\epsilon(\rho_{12}^{12} - \rho^6)
\]

\[
\rho = \frac{\sigma}{h_{12} + \gamma \sigma}
\]

where A1 and A2 are the transformation matrices from the simulation box frame to the body frame and r12 is the center to center vector between the particles. Ur controls the shifted distance dependent interaction based on the distance of closest approach of the two particles (h12) and the user-specified shift parameter gamma. When both particles are spherical, the formula reduces to the usual Lennard-Jones interaction (see details below for when Gay-Berne treats a particle as "spherical").

For large uniform molecules it has been shown that the energy parameters are approximately representable in terms of local contact curvatures (Everaers):
The variable names utilized as potential parameters are for the most part taken from (Everaers) in order to be consistent with the RE-squared pair potential. Details on the upsilon and mu parameters are given here.

More details of the Gay-Berne formulation are given in the references listed below and in this supplementary document.

Use of this pair style requires the NVE, NVT, or NPT fixes with the asphere extension (e.g. fix nve/asphere) in order to integrate particle rotation. Additionally, atom_style ellipsoid should be used since it defines the rotational state and the size and shape of each ellipsoidal particle.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- \( \epsilon_a = \sigma \cdot \frac{a}{b \cdot c} \)
- \( \epsilon_b = \sigma \cdot \frac{b}{a \cdot c} \)
- \( \epsilon_c = \sigma \cdot \frac{c}{a \cdot b} \)

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used.

It is typical with the Gay-Berne potential to define \( \sigma \) as the minimum of the 3 shape diameters of the particles involved in an I,I interaction, though this is not required. Note that this is a different meaning for \( \sigma \) than the pair_style resquered potential uses.

The \( \epsilon_i \) and \( \epsilon_j \) coefficients are actually defined for atom types, not for pairs of atom types. Thus, in a series of pair_coeff commands, they only need to be specified once for each atom type.

Specifically, if any of \( \epsilon_i_a, \epsilon_i_b, \epsilon_i_c \) are non-zero, the three values are assigned to atom type I. If all the \( \epsilon_i \) values are zero, they are ignored. If any of \( \epsilon_j_a, \epsilon_j_b, \epsilon_j_c \) are non-zero, the three values are assigned to atom type J. If all three \( \epsilon_i \) values are zero, they are ignored. Thus the typical way to define the \( \epsilon_i \) and \( \epsilon_j \) coefficients is to list their values in "pair_coeff I J" commands when \( I = J \), but set them to 0.0 when \( I \neq J \). If you do list them when \( I \neq J \), you should insure they are consistent with their values in other pair_coeff commands.

Note that if this potential is being used as a sub-style of pair_style hybrid, and there is no "pair_coeff I I" setting made for Gay-Berne for a particular type I (because I-I interactions are computed by another hybrid pair potential), then you still need to insure the \( \epsilon_a, \epsilon_b, \epsilon_c \) coefficients are assigned to that type in a "pair_coeff I J" command.
IMPORTANT NOTE: If the epsilon \( a = b = c \) for an atom type, and if the shape of the particle itself is spherical, meaning its 3 shape parameters are all the same, then the particle is treated as an LJ sphere by the Gay-Berne potential. This is significant because if two LJ spheres interact, then the simple Lennard-Jones formula is used to compute their interaction energy/force using the specified epsilon and sigma as the standard LJ parameters. This is much cheaper to compute than the full Gay-Berne formula. To treat the particle as a LJ sphere with sigma = \( D \), you should normally set epsilon \( a = b = c = 1.0 \), set the pair_coeff sigma = \( D \), and also set the 3 shape parameters for the particle to \( D \). The one exception is that if the 3 shape parameters are set to 0.0, which is a valid way in LAMMPS to specify a point particle, then the Gay-Berne potential will treat that as shape parameters of 1.0 (i.e. a LJ particle with sigma = 1), since it requires finite-size particles. In this case you should still set the pair_coeff sigma to 1.0 as well.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I \(!= J\), the epsilon and sigma coefficients and cutoff distance for this pair style can be mixed. The default mix value is `geometric`. See the "pair_modify" command for details.

This pair styles supports the `pair_modify` shift option for the energy of the Lennard-Jones portion of the pair interaction, but only for sphere-sphere interactions. There is no shifting performed for ellipsoidal interactions due to the anisotropic dependence of the interaction.

The `pair_modify` table option is not relevant for this pair style.

This pair style does not support the `pair_modify` tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so `pair_style` and `pair_coeff` commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner`, `middle`, `outer` keywords.

**Restrictions:**

The `gayberne` style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

These pair style require that atoms store torque and a quaternion to represent their orientation, as defined by the `atom_style`. It also require they store a per-type shape. The particles cannot store a per-particle diameter.
This pair style requires that atoms be ellipsoids as defined by the `atom_style ellipsoid` command.

Particles acted on by the potential can be extended aspherical or spherical particles, or point particles. Spherical particles have all 3 of their shape parameters equal to each other. Point particles have all 3 of their shape parameters equal to 0.0.

The Gay-Berne potential does not become isotropic as \( r \) increases \((\text{Everaers})\). The distance-of-closest-approach approximation used by LAMMPS becomes less accurate when high-aspect ratio ellipsoids are used.

**Related commands:**

`pair_coeff`, `fix nve/asphere`, `compute temp/asphere`, `pair_style resquared`

**Default:** none


pair_style gran/hooke command
pair_style gran/cuda command
pair_style gran/omp command
pair_style gran/hooke/history command
pair_style gran/hooke/history/omp command
pair_style gran/hertz/history command
pair_style gran/hertz/history/omp command

Syntax:

```
pair_style style Kn Kt gamma_n gamma_t xmu dampflag
```

- **style** = `gran/hooke` or `gran/hooke/history` or `gran/hertz/history`
- **Kn** = elastic constant for normal particle repulsion (force/distance units or pressure units - see discussion below)
- **Kt** = elastic constant for tangential contact (force/distance units or pressure units - see discussion below)
- **gamma_n** = damping coefficient for collisions in normal direction (1/time units or 1/time-distance units - see discussion below)
- **gamma_t** = damping coefficient for collisions in tangential direction (1/time units or 1/time-distance units - see discussion below)
- **xmu** = static yield criterion (unitless fraction between 0.0 and 1.0)
- **dampflag** = 0 or 1 if tangential damping force is excluded or included

IMPORTANT NOTE: Versions of LAMMPS before 9Jan09 had different style names for granular force fields. This is to emphasize the fact that the Hertzian equation has changed to model polydispersity more accurately. A side effect of the change is that the Kn, Kt, gamma_n, and gamma_t coefficients in the pair_style command must be specified with different values in order to reproduce calculations made with earlier versions of LAMMPS, even for monodisperse systems. See the NOTE below for details.

Examples:

```
pair_style gran/hooke/history 200000.0 NULL 50.0 NULL 0.5 1
pair_style gran/hooke 200000.0 70000.0 50.0 30.0 0.5 0
```

Description:

The `gran` styles use the following formulas for the frictional force between two granular particles, as described in (Brilliantov), (Silbert), and (Zhang), when the distance r between two particles of radii Ri and Rj is less than their contact distance d = Ri + Rj. There is no force between the particles when r > d.

The two Hookean styles use this formula:
\[ F_{hk} = (k_n \delta n_{ij} - m_{eff} \gamma_n v_n) - (k_t \Delta s_t + m_{eff} \gamma_t v_t) \]

The Hertzian style uses this formula:

\[ F_{hz} = \sqrt{\delta} \sqrt{\frac{R_i R_j}{R_i + R_j}} F_{hk} = \sqrt{\delta} \sqrt{\frac{R_i R_j}{R_i + R_j}} \left[ (k_n \delta n_{ij} - m_{eff} \gamma_n v_n) - (k_t \Delta s_t + m_{eff} \gamma_t v_t) \right] \]

In both equations the first parenthesized term is the normal force between the two particles and the second parenthesized term is the tangential force. The normal force has 2 terms, a contact force and a damping force. The tangential force also has 2 terms: a shear force and a damping force. The shear force is a "history" effect that accounts for the tangential displacement between the particles for the duration of the time they are in contact. This term is included in pair styles `hooke/history` and `hertz/history`, but is not included in pair style `hooke`. The tangential damping force term is included in all three pair styles if `dampflag` is set to 1; it is not included if `dampflag` is set to 0.

The other quantities in the equations are as follows:

- \( \delta = d - r \) = overlap distance of 2 particles
- \( K_n \) = elastic constant for normal contact
- \( K_t \) = elastic constant for tangential contact
- \( \gamma_n \) = viscoelastic damping constant for normal contact
- \( \gamma_t \) = viscoelastic damping constant for tangential contact
- \( m_{eff} = M_i M_j / (M_i + M_j) \) = effective mass of 2 particles of mass \( M_i \) and \( M_j \)
- \( \Delta \) = tangential displacement vector between 2 spherical particles which is truncated to satisfy a frictional yield criterion
- \( n_{ij} \) = unit vector along the line connecting the centers of the 2 particles
- \( V_n \) = normal component of the relative velocity of the 2 particles
- \( V_t \) = tangential component of the relative velocity of the 2 particles

The \( K_n, K_t, \gamma_n, \) and \( \gamma_t \) coefficients are specified as parameters to the pair_style command. If a NULL is used for \( K_t \), then a default value is used where \( K_t = 2/7 K_n \). If a NULL is used for \( \gamma_t \), then a default value is used where \( \gamma_t = 1/2 \gamma_n \).

The interpretation and units for these 4 coefficients are different in the Hookean versus Hertzian equations.

The Hookean model is one where the normal push-back force for two overlapping particles is a linear function of the overlap distance. Thus the specified \( K_n \) is in units of (force/distance). Note that this push-back force is independent of absolute particle size (in the monodisperse case) and of the relative sizes of the two particles (in the polydisperse case). This model also applies to the other terms in the force equation so that the specified \( \gamma_n \) is in units of (1/time), \( K_t \) is in units of (force/distance), and \( \gamma_t \) is in units of (1/time).

The Hertzian model is one where the normal push-back force for two overlapping particles is proportional to the area of overlap of the two particles, and is thus a non-linear function of overlap distance. Thus \( K_n \) has units of force per area and is thus specified in units of (pressure). The effects of absolute particle size (monodispersity) and relative size (polydispersity) are captured in the radii-dependent pre-factors. When these pre-factors are
carried through to the other terms in the force equation it means that the specified $\gamma_n$ is in units of $(1/(\text{time} \times \text{distance}))$, $K_t$ is in units of (pressure), and $\gamma_t$ is in units of $(1/(\text{time} \times \text{distance}))$.

Note that in the Hookean case, $K_n$ can be thought of as a linear spring constant with units of force/distance. In the Hertzian case, $K_n$ is like a non-linear spring constant with units of force/area or pressure, and as shown in the (Zhang) paper, $K_n = 4G / (3(1-\nu))$ where $\nu$ is the Poisson ratio, $G =$ shear modulus = $E / (2(1+\nu))$, and $E =$ Young's modulus. Similarly, $K_t = 4G / (2-\nu)$. (NOTE: in an earlier version of the manual, we incorrectly stated that $K_t = 8G / (2-\nu)$.)

Thus in the Hertzian case $K_n$ and $K_t$ can be set to values that corresponds to properties of the material being modeled. This is also true in the Hookean case, except that a spring constant must be chosen that is appropriate for the absolute size of particles in the model. Since relative particle sizes are not accounted for, the Hookean styles may not be a suitable model for polydisperse systems.

IMPORTANT NOTE: In versions of LAMMPS before 9Jan09, the equation for Hertzian interactions did not include the $\sqrt{(R_iR_j/R_i+R_j)}$ term and thus was not as accurate for polydisperse systems. For monodisperse systems, $\sqrt{(R_iR_j/R_i+R_j)}$ is a constant factor that effectively scales all 4 coefficients: $K_n$, $K_t$, $\gamma_n$, $\gamma_t$. Thus you can set the values of these 4 coefficients appropriately in the current code to reproduce the results of a previous Hertzian monodisperse calculation. For example, for the common case of a monodisperse system with particles of diameter 1, all 4 of these coefficients should now be set 2x larger than they were previously.

$x_m$ is also specified in the pair_style command and is the upper limit of the tangential force through the Coulomb criterion $F_t = x_m F_n$, where $F_t$ and $F_n$ are the total tangential and normal force components in the formulas above. Thus in the Hookean case, the tangential force between 2 particles grows according to a tangential spring and dash-pot model until $F_t/F_n = x_m$ and is then held at $F_t = F_n x_m$ until the particles lose contact. In the Hertzian case, a similar analogy holds, though the spring is no longer linear.

For granular styles there are no additional coefficients to set for each pair of atom types via the pair_coeff command. All settings are global and are made via the pair_style command. However you must still use the pair_coeff for all pairs of granular atom types. For example the command

\begin{verbatim}
pair_coeff * *
\end{verbatim}

should be used if all atoms in the simulation interact via a granular potential (i.e. one of the pair styles above is used). If a granular potential is used as a sub-style of pair_style hybrid, then specific atom types can be used in the pair_coeff command to determine which atoms interact via a granular potential.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.
Mixing, shift, table, tail correction, restart, rRESPA info:

The pair_modify mix, shift, table, and tail options are not relevant for granular pair styles.

These pair styles write their information to binary restart files, so a pair_style command does not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the pair keyword of the run_style respa command. They do not support the inner, middle, outer keywords.

The single() function of these pair styles returns 0.0 for the energy of a pairwise interaction, since energy is not conserved in these dissipative potentials. It also returns only the normal component of the pairwise interaction force. However, the single() function also calculates 4 extra pairwise quantities. The first 3 are the components of the tangential force between particles I and J, acting on particle I. \( P4 \) is the magnitude of this tangential force. These extra quantities can be accessed by the compute pair/local command, as \( p1, p2, p3, p4 \).

Restrictions: none

All the granular pair styles are part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

These pair styles require that atoms store torque and angular velocity (omega) as defined by the atom_style. They also require a per-particle radius is stored. The sphere atom style does all of this.

This pair style requires you to use the communicate vel yes option so that velocities are stored by ghost atoms.

These pair styles will not restart exactly when using the read_restart command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the read_restart command for more details.

Related commands:

pair_coeff

Default: none


pair_style lj/gromacs command

pair_style lj/gromacs/cuda command

pair_style lj/gromacs/omp command

pair_style lj/gromacs/coul/gromacs command

pair_style lj/gromacs/coul/gromacs/cuda command

pair_style lj/gromacs/coul/gromacs/omp command

Syntax:

pair_style style args

- style = lj/gromacs or lj/gromacs/coul/gromacs
- args = list of arguments for a particular style

lj/gromacs args = inner outer
inner, outer = global switching cutoffs for Lennard Jones
lj/gromacs/coul/gromacs args = inner outer (inner2) (outer2)
inner, outer = global switching cutoffs for Lennard Jones (and Coulombic if only 2 args)
inner2, outer2 = global switching cutoffs for Coulombic (optional)

Examples:

pair_style lj/gromacs 9.0 12.0
pair_coeff * * 100.0 2.0
pair_coeff 2 2 100.0 2.0 8.0 10.0

pair_style lj/gromacs/coul/gromacs 9.0 12.0
pair_style lj/gromacs/coul/gromacs 8.0 10.0 7.0 9.0
pair_coeff * * 100.0 2.0

Description:

The lj/gromacs styles compute shifted LJ and Coulombic interactions with an additional switching function S(r) that ramps the energy and force smoothly to zero between an inner and outer cutoff. It is a commonly used potential in the GROMACS MD code and for the coarse-grained models of Marrink.)
$$E_{LJ} = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] + S_{LJ}(r) \quad r < r_c$$

$$E_C = -\frac{Cq_i q_j}{\epsilon r} + S_C(r) \quad r < r_c$$

$$S'(r) = C \quad r < r_1$$

$$S'(r) = \frac{A}{3} (r - r_1)^3 + \frac{B}{4} (r - r_1)^4 + C \quad r_1 < r < r_c$$

$R_1$ is the inner cutoff; $R_c$ is the outer cutoff. The coefficients $A$, $B$, and $C$ are computed by LAMMPS to perform the shifting and smoothing. The function $S(r)$ is actually applied once to each term of the LJ formula and once to the Coulombic formula, so there are 2 or 3 sets of $A$, $B$, $C$ coefficients depending on which pair_style is used. The boundary conditions applied to the smoothing function are as follows: $S(r_1) = S'(r_1) = 0$, $S(r_c) = -F(r_c)$, $S'(r_c) = -F'(r_c)$, where $F(r)$ is the corresponding term in the LJ or Coulombic potential energy function and a single quote represents a derivative with respect to $r$.

The inner and outer cutoff for the LJ and Coulombic terms can be the same or different depending on whether 2 or 4 arguments are used in the pair_style command. The inner LJ cutoff must be $> 0$, but the inner Coulombic cutoff can be $>= 0$.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- inner (distance units)
- outer (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at $2^{(1/6)}$ sigma.

The last 2 coefficients are optional inner and outer cutoffs for style lj/gromacs. If not specified, the global inner and outer values are used.

The last 2 coefficients cannot be used with style lj/gromacs/coul/gromacs because this force field does not allow varying cutoffs for individual atom pairs; all pairs use the global cutoff(s) specified in the pair_style command.

---

**Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.**

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.
You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the
-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input
script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair
styles can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

None of the GROMACS pair styles support the pair_modify shift option, since the Lennard-Jones portion of the
pair interaction is already smoothed to 0.0 at the cutoff.

The pair_modify table option is not relevant for this pair style.

None of the GROMACS pair styles support the pair_modify tail option for adding long-range tail corrections to
energy and pressure, since there are no corrections for a potential that goes to 0.0 at the cutoff.

All of the GROMACS pair styles write their information to binary restart files, so pair_style and pair_coeff
commands do not need to be specified in an input script that reads a restart file.

All of the GROMACS pair styles can only be used via the pair keyword of the run_style respa command. They do
not support the inner, middle, outer keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

**pair_style hbond/dreiding/lj command**

**pair_style hbond/dreiding/lj/omp command**

**pair_style hbond/dreiding/morse command**

**pair_style hbond/dreiding/morse/omp command**

**Syntax:**

```
pair_style style N inner_distance_cutoff outer_distance_cutoff angle_cutoff
```

- `style` = `hbond/dreiding/lj` or `hbond/dreiding/morse`
- `n` = cosine angle periodicity
- `inner_distance_cutoff` = global inner spline cutoff for Donor-Acceptor interactions (distance units)
- `outer_distance_cutoff` = global cutoff for Donor-Acceptor interactions (distance units)
- `angle_cutoff` = global angle cutoff for Acceptor-Hydrogen-Donor interactions (degrees)

**Examples:**

```plaintext
pair_style hbond/dreiding/lj 4 4.5 5.0 90
pair_coeff * * 3 i 100.0 3.1
pair_coeff * * 2*5 i 100.0 3.1 2 15.0 20.0 135.0

pair_style hbond/dreiding/morse 2 3.0 4.6 75.0
pair_coeff * * 3 j 100.0 1.0 2.0
pair_coeff * * 2*5 j 100.0 1.0 2.0 4.0 6.0
```

**Description:**

The `hbond/dreiding` styles compute the Acceptor-Hydrogen-Donor (AHD) 3-body hydrogen bond interaction for the DREIDING force field, given by:
\[ E = \begin{cases} [LJ(r) | Morse(r)] & r < r_{in} \\ S(r) * [LJ(r) | Morse(r)] & r_{in} < r < r_{out} \\ 0 & r > r_{out} \end{cases} \]

\[ LJ(r) = AR^{-12} - BR^{-10} \cos^n \theta = \epsilon \left\{ 5 \left[ \frac{\sigma}{r} \right]^{12} - 6 \left[ \frac{\sigma}{r} \right]^{10} \right\} \cos^n \theta \]

\[ Morse(r) = D_0 \left\{ \chi^2 - 2\chi \right\} \cos^n \theta = D_0 \left\{ e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right\} \cos^n \theta \]

\[ S(r) = \frac{[r_{out}^2 - r^2]^2 [r_{out}^2 + 2r^2 - 3r_{in}^2]}{[r_{out}^2 - r_{in}^2]^3} \]

where \( r_{in} \) is the inner spline distance cutoff, \( r_{out} \) is the outer distance cutoff, \( \theta_{\text{c}} \) is the angle cutoff, and \( n \) is the cosine periodicity.

Here, \( r \) is the radial distance between the donor (D) and acceptor (A) atoms and \( \theta \) is the bond angle between the acceptor, the hydrogen (H) and the donor atoms:

These 3-body interactions can be defined for pairs of acceptor and donor atoms, based on atom types. For each donor/acceptor atom pair, the 3rd atom in the interaction is a hydrogen permanently bonded to the donor atom, e.g. in a bond list read in from a data file via the read_data command. The atom types of possible hydrogen atoms for each donor/acceptor type pair are specified by the pair_coeff command (see below).

Style \textit{hbond/dreiding/lj} is the original DREIDING potential of (Mayo). It uses a LJ 12/10 functional for the Donor-Acceptor interactions. To match the results in the original paper, use \( n = 4 \).

Style \textit{hbond/dreiding/morse} is an improved version using a Morse potential for the Donor-Acceptor interactions. (Liu) showed that the Morse form gives improved results for Dendrimer simulations, when \( n = 2 \).

See this \textit{howto section} of the manual for more information on the DREIDING forcefield.
Because the Dreiding hydrogen bond potential is only one portion of an overall force field which typically includes other pairwise interactions, it is common to use it as a sub-style in a pair_style hybrid or hybrid/overlay command.

The following coefficients must be defined for pairs of eligible donor/acceptor types via the pair_coeff command as in the examples above.

IMPORTANT NOTE: Unlike other pair styles and their associated pair_coeff commands, you do not need to specify pair_coeff settings for all possible I,J type pairs. Only I,J type pairs for atoms which act as joint donors/acceptors need to be specified; all other type pairs are assumed to be inactive.

IMPORTANT NOTE: A pair_coeff command can be specified multiple times for the same donor/acceptor type pair. This enables multiple hydrogen types to be assigned to the same donor/acceptor type pair. For other pair_styles, if the pair_coeff command is re-used for the same I,J type pair, the settings for that type pair are overwritten. For the hydrogen bond potentials this is not the case; the settings are cumulative. This means the only way to turn off a previous setting, is to re-use the pair_style command and start over.

For the hbond/dreiding/lj style the list of coefficients is as follows:

- K = hydrogen atom type = 1 to Ntypes
- donor flag = i or j
- epsilon (energy units)
- sigma (distance units)
- n = exponent in formula above
- distance cutoff (distance units)
- angle cutoff (degrees)

For the hbond/dreiding/morse style the list of coefficients is as follows:

- K = hydrogen atom type = 1 to Ntypes
- donor flag = i or j
- D0 (energy units)
- alpha (1/distance units)
- r0 (distance units)
- n = exponent in formula above
- distance cutoff (distance units)
- angle cutoff (degrees)

A single hydrogen atom type K can be specified, or a wild-card asterisk can be used in place of or in conjunction with the K arguments to select multiple types as hydrogens. This takes the form "*" or "*n" or "n*" or "m*n". See the pair_coeff command doc page for details.

If the donor flag is i, then the atom of type I in the pair_coeff command is treated as the donor, and J is the acceptor. If the donor flag is j, then the atom of type J in the pair_coeff command is treated as the donor and I is the donor. This option is required because the pair_coeff command requires that I <= J.

Epsilon and sigma are settings for the hydrogen bond potential based on a Lennard-Jones functional form. Note that sigma is defined as the zero-crossing distance for the potential, not as the energy minimum at $2^{(1/6)}$ sigma.

D0 and alpha and r0 are settings for the hydrogen bond potential based on a Morse functional form.

The last 3 coefficients for both styles are optional. If not specified, the global n, distance cutoff, and angle cutoff
specified in the pair_style command are used. If you wish to only override the 2nd or 3rd optional parameter, you must also specify the preceding optional parameters.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `--suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. You must explicitly identify each donor/acceptor type pair.

These styles do not support the `pair_modify` shift option for the energy of the interactions.

The `pair_modify` table option is not relevant for these pair styles.

These pair styles do not support the `pair_modify` tail option for adding long-range tail corrections to energy and pressure.

These pair styles do not write their information to binary restart files, so pair_style and pair_coeff commands need to be re-specified in an input script that reads a restart file.

These pair styles can only be used via the `pair` keyword of the `run_style respa` command. They do not support the `inner`, `middle`, `outer` keywords.

These pair styles tally a count of how many hydrogen bonding interactions they calculate each timestep and the hbond energy. These quantities can be accessed via the `compute pair` command as a vector of values of length 2.

To print these quantities to the log file (with a descriptive column heading) the following commands could be included in an input script:

```
compute hb all pair hbond/dreiding/lj
variable n_hbond equal c_hb[1] #number hbonds
variable E_hbond equal c_hb[2] #hbond energy
thermo_style custom step temp epair v_E_hbond
```

Restrictions: none

Related commands:

pair_coeff

Default: none

pair_style hybrid command

pair_style hybrid/omp command

pair_style hybrid/overlay command

pair_style hybrid/overlay/omp command

Syntax:

pair_style hybrid style1 args style2 args ...
pair_style hybrid/overlay style1 args style2 args ...

- style1,style2 = list of one or more pair styles and their arguments

Examples:

pair_style hybrid lj/cut/coul/cut 10.0 eam lj/cut 5.0
pair_coeff 1*2 1*2 eam niu3
pair_coeff 3 3 lj/cut/coul/cut 1.0 1.0
pair_coeff 1*2 3 lj/cut 0.5 1.2

pair_style hybrid/overlay lj/cut 2.5 coul/long 2.0
pair_coeff * * lj/cut 1.0 1.0
pair_coeff * * coul/long

Description:

The hybrid and hybrid/overlay styles enable the use of multiple pair styles in one simulation. With the hybrid style, exactly one pair style is assigned to each pair of atom types. With the hybrid/overlay style, one or more pair styles can be assigned to each pair of atom types. The assignment of pair styles to type pairs is made via the pair_coeff command.

Here are two examples of hybrid simulations. The hybrid style could be used for a simulation of a metal droplet on a LJ surface. The metal atoms interact with each other via an eam potential, the surface atoms interact with each other via a lj/cut potential, and the metal/surface interaction is also computed via a lj/cut potential. The hybrid/overlay style could be used as in the 2nd example above, where multiple potentials are superposed in an additive fashion to compute the interaction between atoms. In this example, using lj/cut and coul/long together gives the same result as if the lj/cut/coul/long potential were used by itself. In this case, it would be more efficient to use the single combined potential, but in general any combination of pair potentials can be used together in to produce an interaction that is not encoded in any single pair_style file, e.g. adding Coulombic forces between granular particles.

All pair styles that will be used are listed as "sub-styles" following the hybrid or hybrid/overlay keyword, in any order. Each sub-style's name is followed by its usual arguments, as illustrated in the example above. See the doc pages of individual pair styles for a listing and explanation of the appropriate arguments.

Note that an individual pair style can be used multiple times as a sub-style. For efficiency this should only be done if your model requires it. E.g. if you have different regions of Si and C atoms and wish to use a Tersoff potential for pure Si for one set of atoms, and a Tersoff potential for pure C for the other set (presumably with some 3rd potential for Si-C interactions), then the sub-style tersoff could be listed twice. But if you just want to
use a Lennard-Jones or other pairwise potential for several different atom type pairs in your model, then you should just list the sub-style once and use the pair_coeff command to assign parameters for the different type pairs.

IMPORTANT NOTE: An exception to this option to list an individual pair style multiple times are the pair styles implemented as Fortran libraries: pair_style meam and pair_style reax (pair_style reax/c is OK). This is because unlike a C++ class, they can not be instantiated multiple times, due to the manner in which they were coded in Fortran.

In the pair_coeff commands, the name of a pair style must be added after the I,J type specification, with the remaining coefficients being those appropriate to that style. If the pair style is used multiple times in the pair_style command with, then an additional numeric argument must also be included which is the number from 1 to M where M is the number of times the sub-style was listed in the pair style command. The extra number indicates which instance of the sub-style these coefficients apply to.

For example, consider a simulation with 3 atom types: types 1 and 2 are Ni atoms, type 3 are LJ atoms with charges. The following commands would set up a hybrid simulation:

```
pair_style hybrid eam/alloy lj/cut/coul/cut 10.0 lj/cut 8.0
pair_coeff * * eam/alloy nialhjea Ni Ni NULL
pair_coeff 3 3 lj/cut/coul/cut 1.0 1.0
pair_coeff 1*2 3 lj/cut 0.8 1.3
```

As an example of using the same pair style multiple times, consider a simulation with 2 atom types. Type 1 is Si, type 2 is C. The following commands would model the Si atoms with Tersoff, the C atoms with Tersoff, and the cross-interactions with Lennard-Jones:

```
pair_style hybrid lj/cut tersoff tersoff
pair_coeff * * tersoff 1 Si.tersoff Si NULL
pair_coeff * * tersoff 2 C.tersoff NULL C
pair_coeff 1 2 lj/cut 1.0 1.5
```

If pair coefficients are specified in the data file read via the read_data command, then the same rule applies. E.g. "eam/alloy" or "lj/cut" must be added after the atom type, for each line in the "Pair Coeffs" section, e.g.

```
Pair Coeffs

1 lj/cut/coul/cut 1.0 1.0
...
```

Note that the pair_coeff command for some potentials such as pair_style eam/alloy includes a mapping specification of elements to all atom types, which in the hybrid case, can include atom types not assigned to the eam/alloy potential. The NULL keyword is used by many such potentials (eam/alloy, Tersoff, AIREBO, etc), to denote an atom type that will be assigned to a different sub-style.

For the hybrid style, each atom type pair I,J is assigned to exactly one sub-style. Just as with a simulation using a single pair style, if you specify the same atom type pair in a second pair_coeff command, the previous assignment will be overwritten.

For the hybrid/overlay style, each atom type pair I,J can be assigned to one or more sub-styles. If you specify the same atom type pair in a second pair_coeff command with a new sub-style, then the second sub-style is added to the list of potentials that will be calculated for two interacting atoms of those types. If you specify the same atom type pair in a second pair_coeff command with a sub-style that has already been defined for that pair of atoms, then the new pair coefficients simply override the previous ones, as in the normal usage of the pair_coeff
command. E.g. these two sets of commands are the same:

```plaintext
pair_style lj/cut 2.5
pair_coeff * * 1.0 1.0
pair_coeff 2 2 1.5 0.8

pair_style hybrid/overlay lj/cut 2.5
pair_coeff * * lj/cut 1.0 1.0
pair_coeff 2 2 lj/cut 1.5 0.8
```

Coefficients must be defined for each pair of atoms types via the `pair_coeff` command as described above, or in the data file or restart files read by the `read_data` or `read_restart` commands, or by mixing as described below.

For both the `hybrid` and `hybrid/overlay` styles, every atom type pair I,J (where I <= J) must be assigned to at least one sub-style via the `pair_coeff` command as in the examples above, or in the data file read by the `read_data`, or by mixing as described below.

If you want there to be no interactions between a particular pair of atom types, you have 3 choices. You can assign the type pair to some sub-style and use the `neigh_modify exclude type` command. You can assign it to some sub-style and set the coefficients so that there is effectively no interaction (e.g. epsilon = 0.0 in a LJ potential). Or, for `hybrid` and `hybrid/overlay` simulations, you can use this form of the `pair_coeff` command in your input script:

```plaintext
pair_coeff      2 3 none
```

or this form in the "Pair Coeffs" section of the data file:

```plaintext
3 none
```

If an assignment to `none` is made in a simulation with the `hybrid/overlay` pair style, it wipes out all previous assignments of that atom type pair to sub-styles.

Note that you may need to use an `atom_style hybrid` command in your input script, if atoms in the simulation will need attributes from several atom styles, due to using multiple pair potentials.

The potential energy contribution to the overall system due to an individual sub-style can be accessed and output via the `compute pair` command.

IMPORTANT: Several of the potentials defined via the `pair_style` command in LAMMPS are really many-body potentials, such as Tersoff, AIREBO, MEAM, ReaxFF, etc. The way to think about using these potentials in a hybrid setting is as follows.

A subset of atom types is assigned to the many-body potential with a single `pair_coeff` command, using "+* *" to include all types and the NULL keywords described above to exclude specific types not assigned to that potential. If types 1,3,4 were assigned in that way (but not type 2), this means that all many-body interactions between all atoms of types 1,3,4 will be computed by that potential. Pair_style hybrid allows interactions between type pairs 2-2, 1-2, 2-3, 2-4 to be specified for computation by other pair styles. You could even add a second interaction for 1-1 to be computed by another pair style, assuming pair_style hybrid/overlay is used.

But you should not, as a general rule, attempt to exclude the many-body interactions for some subset of the type pairs within the set of 1,3,4 interactions, e.g. exclude 1-1 or 1-3 interactions. That is not conceptually well-defined for many-body interactions, since the potential will typically calculate energies and forces for small groups of atoms, e.g. 3 or 4 atoms, using the neighbor lists of the atoms to find the additional atoms in the group. It is typically non-physical to think of excluding an interaction between a particular pair of atoms when the potential
computes 3-body or 4-body interactions.

However, you can still use the pair_coeff none setting or the neigh_modify exclude command to exclude certain type pairs from the neighbor list that will be passed to a manybody sub-style. This will alter the calculations made by a many-body potential, since it builds its list of 3-body, 4-body, etc interactions from the pair list. You will need to think carefully as to whether it produces a physically meaningful result for your model.

For example, imagine you have two atom types in your model, type 1 for atoms in one surface, and type 2 for atoms in the other, and you wish to use a Tersoff potential to compute interactions within each surface, but not between surfaces. Then either of these two command sequences would implement that model:

```
pair_style hybrid tersoff
pair_coeff * * tersoff SiC.tersoff C C
pair_coeff 1 2 none

pair_style tersoff
pair_coeff * * SiC.tersoff C C
neigh_modify exclude type 1 2
```

Either way, only neighbor lists with 1-1 or 2-2 interactions would be passed to the Tersoff potential, which means it would compute no 3-body interactions containing both type 1 and 2 atoms.

Here is another example, using hybrid/overlay, to use 2 many-body potentials together, in an overlapping manner. Imagine you have CNT (C atoms) on a Si surface. You want to use Tersoff for Si/Si and Si/C interactions, and AIREBO for C/C interactions. Si atoms are type 1; C atoms are type 2. Something like this will work:

```
pair_style hybrid/overlay tersoff airebo 3.0
pair_coeff * * tersoff SiC.tersoff.custom Si C
pair_coeff * * airebo CH.airebo NULL C
```

Note that to prevent the Tersoff potential from computing C/C interactions, you would need to modify the SiC.tersoff file to turn off C/C interaction, i.e. by setting the appropriate coefficients to 0.0.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual.

Since the `hybrid` and `hybrid/overlay` styles delegate computation to the individual sub-styles, the suffix versions of the `hybrid` and `hybrid/overlay` styles are used to propagate the corresponding suffix to all sub-styles, if those versions exist. Otherwise the non-accelerated version will be used.

The individual accelerated sub-styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:
Any pair potential settings made via the `pair_modify` command are passed along to all sub-styles of the hybrid potential.

For atom type pairs I,J and I ≠ J, if the sub-style assigned to I,I and J,J is the same, and if the sub-style allows for mixing, then the coefficients for I,J can be mixed. This means you do not have to specify a `pair_coeff` command for I,J since the IJ type pair will be assigned automatically to the I,I sub-style and its coefficients generated by the mixing rule used by that sub-style. For the `hybrid/overlay` style, there is an additional requirement that both the I,I and J,J pairs are assigned to a single sub-style. See the "pair_modify" command for details of mixing rules. See the See the doc page for the sub-style to see if allows for mixing.

The hybrid pair styles supports the `pair_modify` shift, table, and tail options for an I,J pair interaction, if the associated sub-style supports it.

For the hybrid pair styles, the list of sub-styles and their respective settings are written to binary restart files, so a `pair_style` command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file. Thus, `pair_coeff` commands need to be re-specified in the restart input script.

These pair styles support the use of the `inner`, `middle`, and `outer` keywords of the `run_style respa` command, if their sub-styles do.

**Restrictions:**

When using a long-range Coulombic solver (via the `kspace_style` command) with a hybrid pair_style, one or more sub-styles will be of the "long" variety, e.g. `lj/cut/coul/long` or `buck/coul/long`. You must insure that the short-range Coulombic cutoff used by each of these long pair styles is the same or else LAMMPS will generate an error.

**Related commands:**

`pair_coeff`

**Default:** none
pair_style kim command

Syntax:

pair_style kim virialmode model

- virialmode = KIMvirial or LAMMPSvirial
- model = name of KIM model (potential)

Examples:

pair_style kim KIMvirial model_Ar_P_Morse
pair_coeff * * Ar Ar

Description:

This pair style is a wrapper on the Knowledge Base for Interatomic Models (KIM) repository of interatomic potentials, so that they can be used by LAMMPS scripts.

In KIM lingo, a potential is a "model" and a model contains both the analytic formulas that define the potential as well as the parameters needed to run it for one or more materials, including coefficients and cutoffs.

The argument virialmode determines how the global virial is calculated. If KIMvirial is specified, the KIM model performs the global virial calculation. If LAMMPSvirial is specified, LAMMPS computes the global virial using its fdotr mechanism.

The argument model is the name of the KIM model for a specific potential as KIM defines it. In principle, LAMMPS can invoke any KIM model. You should get an error or warning message from either LAMMPS or KIM if there is an incompatibility.

Only a single pair_coeff command is used with the kim style which specifies the mapping of LAMMPS atom types to KIM elements. This is done by specifying N additional arguments after the * * in the pair_coeff command, where N is the number of LAMMPS atom types:

- N element names = mapping of KIM elements to atom types

As an example, imagine the KIM model supports Si and C atoms. If your LAMMPS simulation has 4 atom types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

pair_coeff * * Si Si Si C

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to Si as defined within KIM. The final C argument maps LAMMPS atom type 4 to C as defined within KIM. If a mapping value is specified as NULL, the mapping is not performed. This can only be used when a kim potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

In addition to the usual LAMMPS error messages, the KIM library itself may generate errors, which should be printed to the screen. In this case it is also useful to check the kim.log file for additional error information. This file kim.log should be generated in the same directory where LAMMPS is running.
Here is information on how to build KIM for use with LAMMPS. There is a directory src/KIM/ with an important file in it: Makefile.lammps. When you do 'make yes-kim' LAMMPS will use the settings in src/KIM/Makefile.lammps to find KIM header files and the KIM library itself for linking purposes. Thus, you should ensure Makefile.lammps has the correct settings for your system and your build of KIM.

Consult the KIM documentation for further details on KIM specifics.

OpenKIM is available for download from this site, namely http://openkim.org. The tarball you download is "openkim-api-vX.X.X.tgz", which can be unpacked via

```
tar xvfz openkim*tgz
```

The openkim/DOCs directory has further documentation. For more information on installing KIM and troubleshooting refer to openkim/INSTALL.

Here is a brief summary of how to build KIM:

1. Set the following environment variables. It is recommended to place the above environment variables definitions in your shell setup file which is located in your home directory (e.g. ~/.bashrc).

   (a) Define the location of the openKIM API root directory. For example, if you untarred the 'openkim-api-vX.X.X.tgz' tarball in your home directory, you would do:

   
   **bash:**
   
   ```
   % export KIM_DIR=~/openkim-api-vX.X.X
   ```
   
   **tcsh:**
   
   ```
   % setenv KIM_DIR ~/openkim-api-vX.X.X
   ```
   
   The '% symbols represent the bash sell prompt and should not be typed.

   (b) By default, all makefiles use the GNU compilers for 64 bit Linux. In order to use the Intel compiler, define the environment variable KIM_INTEL

   **bash:**
   
   ```
   % export KIM_INTEL="yes"
   ```
   
   **tcsh:**
   
   ```
   % setenv KIM_INTEL "yes"
   ```

   (c) For a 32 bit machine, define the environment variable KIM_SYSTEM32

   **bash:**
   
   ```
   % export KIM_SYSTEM32="yes"
   ```
   
   **tcsh:**
   
   ```
   % setenv KIM_SYSTEM32 "yes"
   ```

   (d) Define variable for dynamic linking (recommended)

   **bash:**
   
   ```
   export KIM_DYNAMIC=yes
   ```
tcsh:
setenv KIM_DYNAMIC=yes

If this environment variable is not set the default will be static linking. In that case all KIM models will be linked, producing potentially a very large executable file. It is also possible to build KIM with only a subset of models or a single model you wish to use with LAMMPS. Consult the KIM documentation for details.

2. To compile the package, go to the $KIM_DIR directory and execute make.

```bash
% cd $KIM_DIR
% make examples
% make
```

This builds all Models, Tests, and the openKIM API service routine library. The targets defined by the Makefile in this directory include:

- `make` -- compiles the API and all Models and Tests
- `make all` -- same as `make`
- `make examples` -- copy examples into the appropriate directories
  (no overwrite)
- `make examples-force` -- copy examples into the appropriate directories
  (overwrite)
- `make openkim-api` -- compiles only the API
- `make clean` -- will remove .o, .mod, .a, .so and executable files
- `make examples-clean` -- remove all examples from the MODEL_DRIVERS, MODELS, and TESTs directories.

3. Verify that the compilation was successful by running a Test.

The provided example Tests read in the name of a Model (or Models) which they use to perform their calculations. For most Tests the name of the Model can be piped in using an `echo` command. For example, the following Fortran 90 Test reads in one Model:

```bash
% cd $KIM_DIR/TESTs/test_Ar_free_cluster_CLUSTER_F90
% echo "model_Ar_P_MLJ_CLUSTER_C" | ./test_Ar_free_cluster_CLUSTER_F90
```

(See the README files in the Test directories for an explanation of what the Tests do.)

4. Each Test (and Model) has its own make file for compiling and linking. If changes are made to the code, re-compile (from the $KIM_DIR directory).

5. In case of using a non-standard location for any of the directories KIM_API, TESTs, MODEL_DRIVERS, or MODELS one or more of the following environment variables must be set:

- `KIM_API_DIR`
- `KIM_TESTS_DIR`
- `KIM_MODEL_DRIVERS_DIR`
- `KIM_MODELS_DIR`

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the `pair_modify` mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since KIM stores the potential parameters. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner`, `middle`, `outer` keywords.
Restrictions:

This pair style is part of the KIM package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This current version of pair_style kim is compatible with the openkim-api package version 1.1.0 and higher.

Related commands:

pair_coeff

Default: none
pair_style lcbop command

Syntax:

pair_style lcbop

Examples:

pair_style lcbop
pair_coeff * * ../potentials/C.lcbop C

Description:

The lcbop pair style computes the long-range bond-order potential for carbon (LCBOP) of (Los and Fasolino). See section II in that paper for the analytic equations associated with the potential.

Only a single pair_coeff command is used with the lcbop style which specifies an LCBOP potential file with parameters for specific elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of LCBOP elements to atom types

As an example, if your LAMMPS simulation has 4 atom types and you want the 1st 3 to be C you would use the following pair_coeff command:

pair_coeff * * C.lcbop C C C NULL

The 1st 2 arguments must be ** so as to span all LAMMPS atom types. The first C argument maps LAMMPS atom type 1 to the C element in the LCBOP file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a lcbop potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The parameters/coefficients for the LCBOP potential as applied to C are listed in the C.lcbop file to agree with the original (Los and Fasolino) paper. Thus the parameters are specific to this potential and the way it was fit, so modifying the file should be done carefully.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This pair styles is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.
This pair potential requires the newton setting to be "on" for pair interactions.

The C.lcbop potential file provided with LAMMPS (see the potentials directory) is parameterized for metal units. You can use the LCBOP potential with any LAMMPS units, but you would need to create your own LCBOP potential file with coefficients listed in the appropriate units if your simulation doesn’t use "metal" units.

**Related commands:**

pair_airebo, pair_coeff

**Default:** none

pair_style line/lj command

pair_style line/lj/omp command

Syntax:

pair_style line/lj cutoff

cutoff = global cutoff for interactions (distance units)

Examples:

pair_style line/lj 3.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.5 2.5

Description:

Style line/lj treats particles which are line segments as a set of small spherical particles that tile the line segment length as explained below. Interactions between two line segments, each with N1 and N2 spherical particles, are calculated as the pairwise sum of N1*N2 Lennard-Jones interactions. Interactions between a line segment with N spherical particles and a point particle are treated as the pairwise sum of N Lennard-Jones interactions. See the pair_style lj/cut doc page for the definition of Lennard-Jones interactions.

The cutoff distance for an interaction between 2 line segments, or between a line segment and a point particle, is calculated from the position of the line segment (its center), not between pairs of individual spheres comprising the line segment. Thus an interaction is either calculated in its entirety or not at all.

The set of non-overlapping spherical particles that represent a line segment, for purposes of this pair style, are generated in the following manner. Their size is a function of the line segment length and the specified sigma for that particle type. If a line segment has a length L and is of type I, then the number of spheres N that represent the segment is calculated as N = L/sigma_II, rounded up to an integer value. Thus if L is not evenly divisibly by sigam_II, N is incremented to include one extra sphere. In this case, the spheres must be slightly smaller than sigma_II so as not to overlap, so a new sigma-prime is chosen as the sphere diameter, such that L/N = sigma-prime. Thus the line segment interacts with other segments or point particles as a collection of N spheres of diameter sigma-prime, evenly spaced along the line segment, so as to exactly cover its length.

The LJ interaction between 2 spheres on different line segments of types I,J is computed with an arithmetic mixing of the sigma values of the 2 spheres and using the specified epsilon value for I,J atom types. Note that because the sigma values for line segment spheres is computed using only sigma_II values, specific to the line segment's type, this means that any specified sigma_IJ values (for I != J) are effectively ignored.

For style line/lj, the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)
The last coefficient is optional. If not specified, the global cutoff is used.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of this pair style can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

This pair style does not support the `pair_modify` shift, table, and tail options.

This pair style does not write its information to binary restart files.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner`, `middle`, `outer` keywords.

**Restrictions:**

This style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Defining particles to be line segments so they participate in line/line or line/particle interactions requires the use the `atom_style line` command.

**Related commands:**

`pair_coeff`, `pair_style tri/lj`

**Default:** none
pair_style lj/cut command
pair_style lj/cut/cuda command
pair_style lj/cut/experimental/cuda command
pair_style lj/cut/gpu command
pair_style lj/cut/opt command
pair_style lj/cut/omp command
pair_style lj/cut/coul/cut command
pair_style lj/cut/coul/cut/cuda command
pair_style lj/cut/coul/cut/gpu command
pair_style lj/cut/coul/cut/omp command
pair_style lj/cut/coul/debye command
pair_style lj/cut/coul/debye/cuda command
pair_style lj/cut/coul/debye/gpu command
pair_style lj/cut/coul/debye/omp command
pair_style lj/cut/coul/long command
pair_style lj/cut/coul/long/cuda command
pair_style lj/cut/coul/long/gpu command
pair_style lj/cut/coul/long/opt command
pair_style lj/cut/coul/long/omp command
pair_style lj/cut/coul/long/tip4p command
pair_style lj/cut/coul/long/tip4p/omp command
pair_style lj/cut/coul/long/tip4p/opt command

Syntax:

pair_style style args

- style = lj/cut or lj/cut/coul/cut or lj/cut/coul/debye or lj/cut/coul/long or lj/cut/coul/long/tip4p
- args = list of arguments for a particular style

lj/cut args = cutoff
- cutoff = global cutoff for Lennard Jones interactions (distance units)

lj/cut/coul/cut args = cutoff (cutoff2)
- cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

lj/cut/coul/debye args = kappa cutoff (cutoff2)
- kappa = inverse of the Debye length (inverse distance units)
- cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

lj/cut/coul/long args = cutoff (cutoff2)
- cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

lj/cut/coul/long/tip4p args = otype htype btype atype qdist cutoff (cutoff2)
- otype, htype = atom types for TIP4P O and H
- btype, atype = bond and angle types for TIP4P waters
- qdist = distance from O atom to massless charge (distance units)
- cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

Examples:

pair_style lj/cut 2.5
pair_coeff * * 1 1
pair_coeff 1 1 1.1 2.8

pair_style lj/cut/coul/cut 10.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
pair_coeff 1 1 100.0 3.5 9.0 9.0

pair_style lj/cut/coul/debye 1.5 3.0
pair_coeff * * 100.0 1.0
pair_coeff 1 1 1.0 1.5 2.5
pair_coeff 1 1 1.0 1.5 2.5 5.0

pair_style lj/cut/coul/long 10.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0

pair_style lj/cut/coul/long/tip4p 1 2 7 8 0.15 12.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0

Description:

The lj/cut styles compute the standard 12/6 Lennard-Jones potential, given by
\[ E = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] \quad r < r_c \]

\( r_c \) is the cutoff.

Style \texttt{lj/cut/coul/cut} adds a Coulombic pairwise interaction given by

\[ E = \frac{Cq_i q_j}{\varepsilon r} \quad r < r_c \]

where \( C \) is an energy-conversion constant, \( Q_i \) and \( Q_j \) are the charges on the 2 atoms, and \( \varepsilon \) is the dielectric constant which can be set by the \texttt{dielectric} command. If one cutoff is specified in the \texttt{pair_style} command, it is used for both the LJ and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the LJ and Coulombic terms respectively.

Style \texttt{lj/cut/coul/debye} adds an additional \( \exp() \) damping factor to the Coulombic term, given by

\[ E = \frac{Cq_i q_j}{\varepsilon r} \exp(-\kappa r) \quad r < r_c \]

where \( \kappa \) is the inverse of the Debye length. This potential is another way to mimic the screening effect of a polar solvent.

Style \texttt{lj/cut/coul/long} computes the same Coulombic interactions as style \texttt{lj/cut/coul/cut} except that an additional damping factor is applied to the Coulombic term so it can be used in conjunction with the \texttt{kspace_style} command and its \texttt{ewald} or \texttt{pppm} option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

Style \texttt{lj/cut/coul/long/tip4p} implements the TIP4P water model of (Jorgensen), which introduces a massless site located a short distance away from the oxygen atom along the bisector of the HOH angle. The atomic types of the oxygen and hydrogen atoms, the bond and angle types for OH and HOH interactions, and the distance to the massless charge site are specified as pair_style arguments.

IMPORTANT NOTE: For each TIP4P water molecule in your system, the atom IDs for the O and 2 H atoms must be consecutive, with the O atom first. This is to enable LAMMPS to "find" the 2 H atoms associated with each O atom. For example, if the atom ID of an O atom in a TIP4P water molecule is 500, then its 2 H atoms must have IDs 501 and 502.

See the howto section for more information on how to use the TIP4P pair style. Note that the neighbor list cutoff for Coulomb interactions is effectively extended by a distance 2*qdist when using the TIP4P pair style, to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff \( \geq \) Coulomb cutoff + 2*qdist, to shrink the size of the neighbor list. This leads
to slightly larger cost for the long-range calculation, so you can test the trade-off for your model.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff1 (distance units)
- cutoff2 (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at $2^{(1/6)}$ sigma.

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style lj/cut, since it has no Coulombic terms.

For lj/cut/coul/long and lj/cut/coul/long/tip4p only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual IJ type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles lj/cut/coul/pppm/omp and lj/cut/coul/pppm/tip4p/omp are variants of lj/cut/coul/long/omp and lj/cut/coul/long/tip4p/omp for use with k-space styles pppm/proxy and pppm/tip4p/proxy, respectively and OpenMP multi-threading and will perform the corresponding reciprocal space calculation concurrently with the pair calculation in a separate thread. For certain parallel setups, this may have a performance benefit over performing k-space style and pair style separately and one after the other.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs IJ and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

All of the lj/cut pair styles support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction.
The \textit{lj/cut/coul/long} and \textit{lj/cut/coul/long/tip4p} pair styles support the \texttt{pair\_modify} table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

All of the \textit{lj/cut} pair styles support the \texttt{pair\_modify} tail option for adding a long-range tail correction to the energy and pressure for the Lennard-Jones portion of the pair interaction.

All of the \textit{lj/cut} pair styles write their information to \texttt{binary restart files}, so \texttt{pair\_style} and \texttt{pair\_coeff} commands do not need to be specified in an input script that reads a restart file.

The \textit{lj/cut} and \textit{lj/cut/coul/long} pair styles support the use of the \textit{inner}, \textit{middle}, and \textit{outer} keywords of the \texttt{run\_style respa} command, meaning the pairwise forces can be partitioned by distance at different levels of the \texttt{rRESPA} hierarchy. The other styles only support the \textit{pair} keyword of \texttt{run\_style respa}. See the \texttt{run\_style} command for details.

\textbf{Restrictions:}

The \textit{lj/cut/coul/long} and \textit{lj/cut/coul/long/tip4p} styles are part of the KSPACE package. They are only enabled if LAMMPS was built with those packages. See the \texttt{Making LAMMPS} section for more info. Note that the KSPACE package is installed by default.

\textbf{Related commands:}

\texttt{pair\_coeff}

\textbf{Default:} none

pair_style lj96/cut command

pair_style lj96/cut/cuda command

pair_style lj96/cut/gpu command

pair_style lj96/cut/omp command

Syntax:

pair_style lj96/cut cutoff

- cutoff = global cutoff for lj96/cut interactions (distance units)

Examples:

pair_style lj96/cut 2.5
pair_coeff * * 1.0 1.0 4.0
pair_coeff 1 1 1.0 1.0

Description:

The lj96/cut style computes a 9/6 Lennard-Jones potential, instead of the standard 12/6 potential, given by

$$E = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^9 - \left( \frac{\sigma}{r} \right)^6 \right] \quad r < r_c$$

Rc is the cutoff.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global LJ cutoff specified in the pair_style command is used.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.
You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the
-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input
script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair
styles can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style supports the pair_modify tail option for adding a long-range tail correction to the energy and
pressure of the pair interaction.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to
be specified in an input script that reads a restart file.

This pair style supports the use of the inner, middle, and outer keywords of the run_style respa command,
meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the
run_style command for details.

Restrictions: none

Related commands:

pair_coeff

Default: none
pair_style lj/coul command

pair_style lj/coul/omp command

Syntax:

pair_style lj/coul flag_lj flag_coul cutoff (cutoff2)

- flag_lj = long or cut
  long = use Kspace long-range summation for the dispersion term $1/r^6$
  cut = use a cutoff
- flag_coul = long or off
  long = use Kspace long-range summation for the Coulombic term $1/r$
  off = omit the Coulombic term
- cutoff = global cutoff for LJ (and Coulombic if only 1 cutoff) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

Examples:

pair_style lj/coul cut off 2.5
pair_style lj/coul cut long 2.5 4.0
pair_style lj/coul long long 2.5 4.0
pair_coeff * * 1 1
pair_coeff 1 1 1 3 4

Description:

The lj/coul style computes the standard 12/6 Lennard-Jones and Coulombic potentials, given by

\[
E = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] \quad r < r_c
\]

\[
E = \frac{Cq_iq_j}{\varepsilon r} \quad r < r_c
\]

where C is an energy-conversion constant, Qi and Qj are the charges on the 2 atoms, epsilon is the dielectric constant which can be set by the dielectric command, and Rc is the cutoff. If one cutoff is specified in the pair_style command, it is used for both the LJ and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the LJ and Coulombic terms respectively.

The purpose of this pair style is to capture long-range interactions resulting from both attractive $1/r^6$ Lennard-Jones and Coulombic $1/r$ interactions. This is done by use of the flag_lj and flag_coul settings. The In’t
**Veld** paper has more details on when it is appropriate to include long-range $1/r^6$ interactions, using this potential.

If `flag_lj` is set to `long`, no cutoff is used on the LJ $1/r^6$ dispersion term. The long-range portion is calculated by using the `kspace_style ewald/n` command. The specified LJ cutoff then determines which portion of the LJ interactions are computed directly by the pair potential versus which part is computed in reciprocal space via the Kspace style. If `flag_lj` is set to `cut`, the LJ interactions are simply cutoff, as with `pair_style lj/cut`.

If `flag_coul` is set to `long`, no cutoff is used on the Coulombic interactions. The long-range portion is calculated by using any style, including `ewald/n` of the `kspace_style` command. Note that if `flag_lj` is also set to `long`, then only the `ewald/n` Kspace style can perform the long-range calculations for both the LJ and Coulombic interactions. If `flag_coul` is set to `off`, Coulombic interactions are not computed.

The following coefficients must be defined for each pair of atoms types via the `pair_coeff` command as in the examples above, or in the data file or restart files read by the `read_data` or `read_restart` commands, or by mixing as described below:

- `epsilon` (energy units)
- `sigma` (distance units)
- `cutoff1` (distance units)
- `cutoff2` (distance units)

Note that `sigma` is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at $2^{(1/6)}$ `sigma`.

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the `pair_style` command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair. Note that if you are using `flag_lj` set to `long`, you cannot specify a LJ cutoff for an atom type pair, since only one global LJ cutoff is allowed. Similarly, if you are using `flag_coul` set to `long`, you cannot specify a Coulombic cutoff for an atom type pair, since only one global Coulombic cutoff is allowed.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I !≠ J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is `geometric`. See the "pair_modify" command for details.

This pair style supports the `pair_modify` shift option for the energy of the Lennard-Jones portion of the pair interaction, assuming `flag_lj` is `cut`. 

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.
This pair style supports the pair_modify table option since it can tabulate the short-range portion of the long-range Coulombic interaction.

This pair style does not support the pair_modify tail option for adding a long-range tail correction to the Lennard-Jones portion of the energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style supports the use of the inner, middle, and outer keywords of the run_style respa command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the run_style command for details.

**Restrictions:**

This style is part of the USER-EWALDN package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

pair_coeff

**Default:** none

pair_style lj/cubic command

pair_style lj/cubic/omp command

Syntax:

pair_style lj/cubic

Examples:

pair_style lj/cubic
pair_coeff * * 1.0 0.8908987

Description:

The lj/cubic style computes a truncated LJ interaction potential whose energy and force are continuous everywhere. Inside the inflection point the interaction is identical to the standard 12/6 Lennard-Jones potential. The LJ function outside the inflection point is replaced with a cubic function of distance. The energy, force, and second derivative are continuous at the inflection point. The cubic coefficient A3 is chosen so that both energy and force go to zero at the cutoff distance. Outside the cutoff distance the energy and force are zero.

\[ E = u_{LJ}(r) \quad r \leq r_s \]
\[ = u_{LJ}(r_s) + (r - r_s)u'_{LJ}(r_s) - \frac{1}{6}A_3(r - r_s)^3 \quad r_s < r \leq r_c \]
\[ = 0 \quad r > r_c \]

The location of the inflection point rs is defined by the LJ diameter, rs/\(\sigma\) = \((26/7)^{1/6}\). The cutoff distance is defined by rc/rs = 67/48 or rc/\(\sigma\) = 1.737... The analytic expression for the the cubic coefficient \(A_3r_{min}^3/\varepsilon = 27.93...\) is given in the paper by Holian and Ravelo (Holian).

This potential is commonly used to study the shock mechanics of FCC solids, as in Ravelo et al. (Ravelo).

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- \(\varepsilon\) (energy units)
- \(\sigma\) (distance units)

Note that \(\sigma\) is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum, which is located at \(r_{min} = 2^{(1/6)}\sigma\). In the above example, \(\sigma = 0.8908987\), so \(r_{min} = 1\).

Styles with a \(cuda, gpu, omp, or opt\) suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.
These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

---

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

The lj/cubic pair style does not support the pair_modify shift option, since pair interaction is already smoothed to 0.0 at the cutoff.

The pair_modify table option is not relevant for this pair style.

The lj/cubic pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since there are no corrections for a potential that goes to 0.0 at the cutoff.

The lj/cubic pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The lj/cubic pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

---

**Restrictions:** none

**Related commands:**

pair_coeff

**Default:** none


pair_style lj/cut/smooth command

pair_style lj/cut/smooth/cuda command

pair_style lj/cut/smooth/omp command

Syntax:

pair_style lj/cut/smooth Rc

- Rc = cutoff for lj/cut/smooth interactions (distance units)

Examples:

pair_style lj/cut/smooth 5.456108274435118
pair_coeff * * 0.7242785984051078 2.598146797350056
pair_coeff 1 1 20.0 1.3 9.0

Description:

Style lj/cut/smooth computes a LJ interaction that combines the standard 12/6 Lennard-Jones function and
subtracts a linear term that includes a cutoff distance Rc.

At the cutoff Rc, the energy and force (its 1st derivative) will be 0.0.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the
examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as
described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

If not specified, the global value for Rc is used.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix.
They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate
of the manual. The accelerated styles take the same arguments and should produce the same results, except for
round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They
are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the
-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input
script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.
Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since the energy of the pair interaction is smoothed to 0.0 at the cutoff.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

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pair_style lj/expand command

pair_style lj/expand/cuda command

pair_style lj/expand/gpu command

pair_style lj/expand/omp command

Syntax:

pair_style lj/expand cutoff

  • cutoff = global cutoff for lj/expand interactions (distance units)

Examples:

pair_style lj/expand 2.5
pair_coeff * * 1.0 1.0 0.5
pair_coeff 1 1 1.0 1.0 -0.2 2.0

Description:

Style lj/expand computes a LJ interaction with a distance shifted by delta which can be useful when particles are of different sizes, since it is different that using different sigma values in a standard LJ formula:
\[ E = 4\varepsilon \left[ \left( \frac{\sigma}{r - \Delta} \right)^{12} - \left( \frac{\sigma}{r - \Delta} \right)^{6} \right] \quad r < r_c + \Delta \]

Rc is the cutoff which does not include the delta distance. I.e. the actual force cutoff is the sum of cutoff + delta.

The following coefficients must be defined for each pair of atoms types via the `pair_coeff` command as in the examples above, or in the data file or restart files read by the `read_data` or `read_restart` commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- delta (distance units)
- cutoff (distance units)

The delta values can be positive or negative. The last coefficient is optional. If not specified, the global LJ cutoff is used.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I ≠ J, the epsilon, sigma, and shift coefficients and cutoff distance for this pair style can be mixed. Shift is always mixed via an arithmetic rule. The other coefficients are mixed according to the `pair_modify` mix value. The default mix value is geometric. See the "pair_modify" command for details.

This pair style supports the `pair_modify` shift option for the energy of the pair interaction.

The `pair_modify` table option is not relevant for this pair style.

This pair style supports the `pair_modify` tail option for adding a long-range tail correction to the energy and pressure of the pair interaction.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.
This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

**Restrictions:** none

**Related commands:**

pair_coeff

**Default:** none
pair_style lj/sf command

pair_style lj/sf/omp command

Syntax:

pair_style lj/sf cutoff

• cutoff = global cutoff for Lennard-Jones interactions (distance units)

Examples:

pair_style lj/sf 2.5
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.0 3.0

Description:

Style lj/sf computes a truncated and force-shifted LJ interaction (Shifted Force Lennard-Jones), so that both the potential and the force go continuously to zero at the cutoff (Toxvaerd):

\[
F = F_{\text{LJ}}(r) - F_{\text{LJ}}(r_c) \quad r < r_c
\]
\[
E = E_{\text{LJ}}(r) - E_{\text{LJ}}(r_c) + (r - r_c) F_{\text{LJ}}(r_c) \quad r < r_c
\]

with

\[
E_{\text{LJ}}(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]
\]

and

\[
F_{\text{LJ}}(r) = -E'_{\text{LJ}}(r)
\]

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

• epsilon (energy units)
• sigma (distance units)
• cutoff (distance units)

The last coefficient is optional. If not specified, the global LJ cutoff specified in the pair_style command is used.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.
You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the
-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input
script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for this pair style can be
mixed. Rin is a cutoff value and is mixed like the cutoff. The default mix value is geometric. See the
"pair_modify" command for details.

The pair_modify shift option is not relevant for this pair style, since the pair interaction goes to 0.0 at the cutoff.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and
pressure, since the energy of the pair interaction is smoothed to 0.0 at the cutoff.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to
be specified in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the
inner, middle, outer keywords.

Restrictions:

This pair style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package.
See the Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

pair_style lj/smooth command

pair_style lj/smooth/cuda command

pair_style lj/smooth/omp command

Syntax:

pair_style lj/smooth Rin Rc

- Rin = inner cutoff beyond which force smoothing will be applied (distance units)
- Rc = outer cutoff for lj/smooth interactions (distance units)

Examples:

pair_style lj/smooth 8.0 10.0
pair_coeff * * 10.0 1.5
pair_coeff 1 1 20.0 1.3 7.0 9.0

Description:

Style lj/smooth computes a LJ interaction with a force smoothing applied between the inner and outer cutoff.

\[
E = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] \quad r < r_{in}
\]

\[
F = C_1 + C_2 (r - r_{in}) + C_3 (r - r_{in})^2 + C_4 (r - r_{in})^3 \quad r_{in} < r < r_c
\]

The polynomial coefficients C1, C2, C3, C4 are computed by LAMMPS to cause the force to vary smoothly from the inner cutoff Rin to the outer cutoff Rc.

At the inner cutoff the force and its 1st derivative will match the unsmoothed LJ formula. At the outer cutoff the force and its 1st derivative will be 0.0. The inner cutoff cannot be 0.0.

IMPORTANT NOTE: this force smoothing causes the energy to be discontinuous both in its values and 1st derivative. This can lead to poor energy conservation and may require the use of a thermostat. Plot the energy and force resulting from this formula via the pair_write command to see the effect.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- inner (distance units)
- outer (distance units)
The last 2 coefficients are optional inner and outer cutoffs. If not specified, the global values for Rin and Rc are used.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix command-line switch` when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs IJ and I != J, the epsilon, sigma, Rin coefficients and the cutoff distance for this pair style can be mixed. Rin is a cutoff value and is mixed like the cutoff. The other coefficients are mixed according to the pair_modify mix option. The default mix value is geometric. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since the energy of the pair interaction is smoothed to 0.0 at the cutoff.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions: none

Related commands:

pair_coeff, pair lj/smooth/linear

Default: none
**pair_style lj/smooth/linear command**

**pair_style lj/smooth/linear/omp command**

**Syntax:**

.pair_style lj/smooth/linear Rc

- Rc = cutoff for lj/smooth/linear interactions (distance units)

**Examples:**

.pair_style lj/smooth/linear 5.456108274435118
.pair_coeff * * 0.7242785984051078 2.598146797350056
.pair_coeff 1 1 20.0 1.3 9.0

**Description:**

Style *lj/smooth/linear* computes a LJ interaction that combines the standard 12/6 Lennard-Jones function and subtracts a linear term that includes the cutoff distance Rc, as in this formula:

At the cutoff Rc, the energy and force (its 1st derivative) will be 0.0.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global value for Rc is used.

Styles with a *cuda*, *gpu*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix* command-line switch when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**
For atom type pairs I,J and I !\neq J, the epsilon and sigma coefficients and cutoff distance can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since the energy of the pair interaction is smoothed to 0.0 at the cutoff.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions: none

Related commands:

pair_coeff, pair lj/smooth

Default: none
**pair_style lubricate command**

**pair_style lubricate/omp command**

**pair_style lubricate/poly command**

**pair_style lubricate/poly/omp command**

**Syntax:**

```
pair_style style mu flaglog flagfld cutinner cutoff flagHI flagVF

style = lubricate or lubricate/poly
mu = dynamic viscosity (dynamic viscosity units)
flaglog = 0/1 log terms in the lubrication approximation off/on
flagfld = 0/1 to include/exclude Fast Lubrication Dynamics effects
cutinner = inner cutoff distance (distance units)
cutoff = outer cutoff for interactions (distance units)
flagHI (optional) = 0/1 to include/exclude 1/r hydrodynamic interactions
flagVF (optional) = 0/1 to include/exclude volume fraction corrections in the long-range isotropic terms
```

**Examples:** (all assume radius = 1)

```
pair_style lubricate 1.5 1 1 2.01 2.5
pair_coeff 1 1 2.05 2.8
pair_coeff * *

pair_style lubricate 1.5 1 1 2.01 2.5
pair_coeff * *
variable mu equal ramp(1,2)
fix 1 all adapt 1 pair lubricate mu * * v_mu
```

**Description:**

Styles *lubricate* and *lubricate/poly* compute hydrodynamic interactions between mono-disperse spherical particles in a pairwise fashion. The interactions have 2 components. The first is Ball-Melrose lubrication terms via the formulas in *(Ball and Melrose)*

\[
W = -a_{sq} |(v_1 - v_2) \bullet nn|^{2} - a_{sh} |(\omega_1 + \omega_2) \bullet (I - nn) - 2\Omega_N|^{2} - a_{pu} |(\omega_1 - \omega_2) \bullet (I - nn)|^{2} - a_{tw} |(\omega_1 - \omega_2) \bullet nn|^{2} \quad r < r_c
\]

\[
\Omega_N = n \times (v_1 - v_2)/r
\]
which represents the dissipation $W$ between two nearby particles due to their relative velocities in the presence of a background solvent with viscosity $\mu$. Note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity.

The $A$sq (squeeze) term is the strongest and is included if $flagHI$ is set to 1 (default). It scales as $1/gap$ where gap is the separation between the surfaces of the 2 particles. The $A$sh (shear) and $A$pu (pump) terms are only included if $flaglog$ is set to 1. They are the next strongest interactions, and the only other singular interaction, and scale as $\log(gap)$. Note that $flaglog = 1$ and $flagHI = 0$ is invalid, and will result in a warning message, after which $flagHI$ will be set to 1. The $Atw$ (twist) term is currently not included. It is typically a very small contribution to the lubrication forces.

The $flagHI$ and $flagVF$ settings are optional. Neither should be used, or both must be defined.

$Cutinner$ sets the minimum center-to-center separation that will be used in calculations irrespective of the actual separation. $Cutoff$ is the maximum center-to-center separation at which an interaction is computed. Using a $cutoff$ less than 3 radii is recommended if $flaglog$ is set to 1.

The other component is due to the Fast Lubrication Dynamics (FLD) approximation, described in (Kumar), which can be represented by the following equation

$$F^H = -R_{FU}(U - U^\infty) + R_{FE}E^\infty$$

where $U$ represents the velocities and angular velocities of the particles, $U^\infty$ represents the velocity and the angular velocity of the undisturbed fluid, and $E^\infty$ represents the rate of strain tensor of the undisturbed fluid with viscosity $\mu$. Again, note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity. Volume fraction corrections to $R_{FU}$ are included as long as $flagVF$ is set to 1 (default).

IMPORTANT NOTE: When using the FLD terms, these pair styles are designed to be used with explicit time integration and a correspondingly small timestep. Thus either fix nve/sphere or fix nve/asphere should be used for time integration. To perform implicit FLD, see the pair_style lubricateU command.

Style lubricate requires monodisperse spherical particles; style lubricate/poly allows for polydisperse spherical particles.

The viscosity $\mu$ can be varied in a time-dependent manner over the course of a simulation, in which case in which case the pair_style setting for $\mu$ will be overridden. See the fix adapt command for details.

If the suspension is sheared via the fix deform command then the pair style uses the shear rate to adjust the hydrodynamic interactions accordingly. Volume changes due to fix deform are accounted for when computing the volume fraction corrections to $R_{FU}$.

When computing the volume fraction corrections to $R_{FU}$, the presence of walls (whether moving or stationary) will affect the volume fraction available to colloidal particles. This is currently accounted for with the following types of walls: wall/lj93, wall/lj126, wall/colloid, and wall/harmonic. For these wall styles, the correct volume fraction will be used when walls do not coincide with the box boundary, as well as when walls move and thereby cause a change in the volume fraction. Other wall styles will still work, but they will result in the volume fraction being computed based on the box boundaries.

Since lubrication forces are dissipative, it is usually desirable to thermostat the system at a constant temperature. If Brownian motion (at a constant temperature) is desired, it can be set using the pair_style brownian command.
These pair styles and the brownian style should use consistent parameters for \textit{mu}, \textit{flaglog}, \textit{flagfld}, \textit{cutinner}, \textit{cutoff}, \textit{flagHI} and \textit{flagVF}.

The following coefficients must be defined for each pair of atoms types via the \texttt{pair_coeff} command as in the examples above, or in the data file or restart files read by the \texttt{read_data} or \texttt{read_restart} commands, or by mixing as described below:

- \texttt{cutinner} (distance units)
- \texttt{cutoff} (distance units)

The two coefficients are optional. If neither is specified, the two cutoffs specified in the pair\_style command are used. Otherwise both must be specified.

Styles with a \texttt{cuda}, \texttt{gpu}, \texttt{omp}, or \texttt{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in this section of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \texttt{-suffix} command-line switch when you invoke LAMMPS, or you can use the \texttt{suffix} command in your input script.

See this section of the manual for more instructions on how to use the accelerated styles effectively.

\textbf{Mixing, shift, table, tail correction, restart, rRESPA info:}

For atom type pairs I,J and I \neq J, the two cutoff distances for this pair style can be mixed. The default mix value is \textit{geometric}. See the "pair\_modify" command for details.

This pair style does not support the \texttt{pair\_modify} shift option for the energy of the pair interaction.

The \texttt{pair\_modify} table option is not relevant for this pair style.

This pair style does not support the \texttt{pair\_modify} tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair\_style and pair\_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the \texttt{pair} keyword of the \texttt{run_style respa} command. It does not support the \texttt{inner}, \texttt{middle}, \texttt{outer} keywords.

\textbf{Restrictions:}

These styles are part of the FLD package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Only spherical monodisperse particles are allowed for pair\_style lubricate.
Only spherical particles are allowed for pair_style lubricate/poly.

These pair styles will not restart exactly when using the read_restart command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the read_restart command for more details.

**Related commands:**

pair_coeff, pair_style lubricateU

**Default:**

The default settings for the optional args are flagHI = 1 and flagVF = 1.

---


*(Kumar)* Kumar and Higdon, Phys Rev E, 82, 051401 (2010).
pair_style lubricateU command

pair_style lubricateU/poly command

Syntax:

```
pair_style style mu flaglog cutinner cutoff gdot flagHI flagVF
```

- style = lubricateU or lubricateU/poly
- mu = dynamic viscosity (dynamic viscosity units)
- flaglog = 0/1 log terms in the lubrication approximation on/off
- cutinner = inner cut off distance (distance units)
- cutoff = outer cutoff for interactions (distance units)
- gdot = shear rate (1/time units)
- flagHI (optional) = 0/1 to include/exclude 1/r hydrodynamic interactions
- flagVF (optional) = 0/1 to include/exclude volume fraction corrections in the long-range isotropic terms

Examples: (all assume radius = 1)

```
pair_style lubricateU 1.5 1 2.01 2.5 0.01 1 1
pair_coeff 1 1 2.05 2.8
pair_coeff * *
```

Description:

Styles lubricateU and lubricateU/poly compute velocities and angular velocities such that the hydrodynamic interaction balances the force and torque due to all other types of interactions.

The interactions have 2 components. The first is Ball-Melrose lubrication terms via the formulas in (Ball and Melrose)

\[
W = -a_{sq}|(v_1 - v_2) \cdot nn|^2 - a_{sh}|(\omega_1 + \omega_2) \cdot (I - nn) - 2\Omega_N|^2 - a_{pu}|(\omega_1 - \omega_2) \cdot (I - nn)|^2 - a_{tw}|(\omega_1 - \omega_2) \cdot nn|^2 \quad r < r_c
\]

\[
\Omega_N = n \times (v_1 - v_2)/r
\]

which represents the dissipation W between two nearby particles due to their relative velocities in the presence of a background solvent with viscosity \( \mu \). Note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity.

The Asq (squeeze) term is the strongest and is included as long as flagHI is set to 1 (default). It scales as 1/gap where gap is the separation between the surfaces of the 2 particles. The Ash (shear) and Apu (pump) terms are only included if flaglog is set to 1. They are the next strongest interactions, and the only other singular interaction, and scale as log(gap). Note that flaglog = 1 and flagHI = 0 is invalid, and will result in a warning message, after
which \texttt{flagHI} will be set to 1. The Atw (twist) term is currently not included. It is typically a very small contribution to the lubrication forces.

The \texttt{flagHI} and \texttt{flagVF} settings are optional. Neither should be used, or both must be defined.

\textit{Cutinner} sets the minimum center-to-center separation that will be used in calculations irrespective of the actual separation. \textit{Cutoff} is the maximum center-to-center separation at which an interaction is computed. Using a cutoff less than 3 radii is recommended if \texttt{flaglog} is set to 1.

The other component is due to the Fast Lubrication Dynamics (FLD) approximation, described in (Kumar). The equation being solved to balance the forces and torques is

\[ -R_{FU}(U - U^{\infty}) = -R_{FE}E^{\infty} - F^{rest} \]

where \( U \) represents the velocities and angular velocities of the particles, \( U^{\infty} \) represents the velocities and the angular velocities of the undisturbed fluid, and \( E^{\infty} \) represents the rate of strain tensor of the undisturbed fluid flow with viscosity \( \mu \). Again, note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity. Volume fraction corrections to \( R_{FU} \) are included if \texttt{flagVF} is set to 1 (default).

\( F^{rest} \) represents the forces and torques due to all other types of interactions, e.g. Brownian, electrostatic etc. Note that this algorithm neglects the inertial terms, thereby removing the restriction of resolving the small interal time scale, which may not be of interest for colloidal particles. This pair style solves for the velocity such that the hydrodynamic force balances all other types of forces, thereby resulting in a net zero force (zero inertia limit). When defining this pair style, it must be defined last so that when this style is invoked all other types of forces have already been computed. For the same reason, it won't work if additional non-pair styles are defined (such as bond or Kspace forces) as they are calculated in LAMMPS after the pairwise interactions have been computed.

IMPORTANT NOTE: When using these styles, the these pair styles are designed to be used with implicit time integration and a correspondingly larger timestep. Thus either \texttt{fix nve/noforce} should be used for spherical particles defined via \texttt{atom_style sphere} or \texttt{fix nve/aspHERE/noforce} should be used for spherical particles defined via \texttt{atom_style ellipsoid}. This is because the velocity and angular momentum of each particle is set by the pair style, and should not be reset by the time integration fix.

Style \texttt{lubricateU} requires monodisperse spherical particles; style \texttt{lubricateU/poly} allows for polydisperse spherical particles.

If the suspension is sheared via the \texttt{fix deform} command then the pair style uses the shear rate to adjust the hydrodynamic interactions accordingly. Volume changes due to fix deform are accounted for when computing the volume fraction corrections to \( R_{FU} \).

When computing the volume fraction corrections to \( R_{FU} \), the presence of walls (whether moving or stationary) will affect the volume fraction available to colloidal particles. This is currently accounted for with the following types of walls: \texttt{wall/lj93}, \texttt{wall/lj126}, \texttt{wall/colloid}, and "wall/harmonic fix wall.html". For these wall styles, the correct volume fraction will be used when walls do not coincide with the box boundary, as well as when walls move and thereby cause a change in the volume fraction. To use these wall styles with pair style \texttt{lubricateU} or \texttt{lubricateU/poly}, the \texttt{fld yes} option must be specified in the fix wall command.

Since lubrication forces are dissipative, it is usually desirable to thermostat the system at a constant temperature. If Brownian motion (at a constant temperature) is desired, it can be set using the \texttt{pair_style brownian} command.
These pair styles and the brownian style should use consistent parameters for \textit{mu}, \textit{flaglog}, \textit{flagfld}, \textit{cutinner}, \textit{cutoff}, \textit{flagHI} and \textit{flagVF}.

The following coefficients must be defined for each pair of atoms types via the \texttt{pair\_coeff} command as in the examples above, or in the data file or restart files read by the \texttt{read\_data} or \texttt{read\_restart} commands, or by mixing as described below:

- \textit{cutinner} (distance units)
- \textit{cutoff} (distance units)

The two coefficients are optional. If neither is specified, the two cutoffs specified in the \texttt{pair\_style} command are used. Otherwise both must be specified.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I \neq J, the two cutoff distances for this pair style can be mixed. The default mix value is \textit{geometric}. See the "pair\_modify" command for details.

This pair style does not support the \texttt{pair\_modify} shift option for the energy of the pair interaction.

The \texttt{pair\_modify} table option is not relevant for this pair style.

This pair style does not support the \texttt{pair\_modify} tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so \texttt{pair\_style} and \texttt{pair\_coeff} commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the \textit{pair} keyword of the \texttt{run\_style respa} command. It does not support the \textit{inner, middle, outer} keywords.

**Restrictions:**

These styles are part of the FLD package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Currently, these pair styles assume that all other types of forces/torques on the particles have been already been computed when it is invoked. This requires this style to be defined as the last of the pair styles, and that no fixes apply additional constraint forces. One exception is the \texttt{fix wall/colloid} commands, which has an "fld" option to apply their wall forces correctly.

Only spherical monodisperse particles are allowed for \texttt{pair\_style lubricateU}.

Only spherical particles are allowed for \texttt{pair\_style lubricateU/poly}.

For sheared suspensions, it is assumed that the shearing is done in the xy plane, with x being the velocity direction and y being the velocity-gradient direction. In this case, one must use \texttt{fix deform} with the same rate of shear (erate).

**Related commands:**

\texttt{pair\_coeff}, \texttt{pair\_style lubricate}
Default:

The default settings for the optional args are flagHI = 1 and flagVF = 1.

(Ball) Ball and Melrose, Physica A, 247, 444-472 (1997).

(Kumar) Kumar and Higdon, Phys Rev E, 82, 051401 (2010).
pair_style meam command

Syntax:

pair_style meam

Examples:

pair_style meam
pair_coeff * * ../potentials/library.meam Si ../potentials/si.meam Si
pair_coeff * * ../potentials/library.meam Ni Al NULL Ni Al Ni Ni

Description:

NOTE: The behavior of the MEAM potential for alloy systems has changed as of November 2010; see description below of the mixture_ref_t parameter

Style meam computes pairwise interactions for a variety of materials using modified embedded-atom method (MEAM) potentials (Baskes). Conceptually, it is an extension to the original EAM potentials which adds angular forces. It is thus suitable for modeling metals and alloys with fcc, bcc, hcp and diamond cubic structures, as well as covalently bonded materials like silicon and carbon.

In the MEAM formulation, the total energy $E$ of a system of atoms is given by:

$$E = \sum_i \left\{ F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(r_{ij}) \right\}$$

where $F$ is the embedding energy which is a function of the atomic electron density $\rho$, and $\phi$ is a pair potential interaction. The pair interaction is summed over all neighbors $J$ of atom $I$ within the cutoff distance. As with EAM, the multi-body nature of the MEAM potential is a result of the embedding energy term. Details of the computation of the embedding and pair energies, as implemented in LAMMPS, are given in (Gullet) and references therein.

The various parameters in the MEAM formulas are listed in two files which are specified by the pair_coeff command. These are ASCII text files in a format consistent with other MD codes that implement MEAM potentials, such as the serial DYNAMO code and Warp. Several MEAM potential files with parameters for different materials are included in the "potentials" directory of the LAMMPS distribution with a ".meam" suffix. All of these are parameterized in terms of LAMMPS metal units.

Note that unlike for other potentials, cutoffs for MEAM potentials are not set in the pair_style or pair_coeff command; they are specified in the MEAM potential files themselves.

Only a single pair_coeff command is used with the meam style which specifies two MEAM files and the element(s) to extract information for. The MEAM elements are mapped to LAMMPS atom types by specifying $N$ additional arguments after the 2nd filename in the pair_coeff command, where $N$ is the number of LAMMPS atom types:
As an example, the potentials/library.meam file has generic MEAM settings for a variety of elements. The potentials/sic.meam file has specific parameter settings for a Si and C alloy system. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * library.meam Si C sic.meam Si Si Si C
```

The 1st 2 arguments must be ** so as to span all LAMMPS atom types. The two filenames are for the library and parameter file respectively. The Si and C arguments (between the file names) are the two elements for which info will be extracted from the library file. The first three trailing Si arguments map LAMMPS atom types 1,2,3 to the MEAM Si element. The final C argument maps LAMMPS atom type 4 to the MEAM C element.

If the 2nd filename is specified as NULL, no parameter file is read, which simply means the generic parameters in the library file are used. Use of the NULL specification for the parameter file is discouraged for systems with more than a single element type (e.g. alloys), since the parameter file is expected to set element interaction terms that are not captured by the information in the library file.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when a meam potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The MEAM library file provided with LAMMPS has the name potentials/library.meam. It is the "meamf" file used by other MD codes. Aside from blank and comment lines (start with #) which can appear anywhere, it is formatted as a series of entries, each of which has 19 parameters and can span multiple lines:

- elt, lat, z, ielement, atwt, alpha, b0, b1, b2, b3, alat, esub, asub, t0, t1, t2, t3, rozero, ibar

The "elt" and "lat" parameters are text strings, such as elt = Si or Cu and lat = dia or fcc. Because the library file is used by Fortran MD codes, these strings may be enclosed in single quotes, but this is not required. The other numeric parameters match values in the formulas above. The value of the "elt" string is what is used in the pair_coeff command to identify which settings from the library file you wish to read in. There can be multiple entries in the library file with the same "elt" value; LAMMPS reads the 1st matching entry it finds and ignores the rest.

Other parameters in the MEAM library file correspond to single-element potential parameters:

- lat = lattice structure of reference configuration
- z = number of nearest neighbors in the reference structure
- ielement = atomic number
- atwt = atomic weight
- alat = lattice constant of reference structure
- esub = energy per atom (eV) in the reference structure at equilibrium
- asub = "A" parameter for MEAM (see e.g. (Baskes))

The alpha, b0, b1, b2, b3, t0, t1, t2, t3 parameters correspond to the standard MEAM parameters in the literature (Baskes) (the b parameters are the standard beta parameters). The rozero parameter is an element-dependent density scaling that weights the reference background density (see e.g. equation 4.5 in (Gullet)) and is typically 1.0 for single-element systems. The ibar parameter selects the form of the function G(Gamma) used to compute the electron density; options are
0 => \( G = \sqrt{1+\Gamma} \)
1 => \( G = \exp(\Gamma/2) \)
2 => not implemented
3 => \( G = 2/(1+\exp(-\Gamma)) \)
4 => \( G = \sqrt{1+\Gamma} \)
-5 => \( G = \pm \sqrt{\operatorname{abs}(1+\Gamma)} \)

If used, the MEAM parameter file contains settings that override or complement the library file settings. Examples of such parameter files are in the potentials directory with a ".meam" suffix. Their format is the same as is read by other Fortran MD codes. Aside from blank and comment lines (start with #) which can appear anywhere, each line has one of the following forms. Each line can also have a trailing comment (starting with #) which is ignored.

```plaintext
keyword = value
keyword(I) = value
keyword(I,J) = value
keyword(I,J,K) = value
```

The recognized keywords are as follows:

- \( Ec, \alpha, \rho_0, \delta, \text{lattice}, \text{attrac}, \text{repuls}, \text{nn2}, \text{Cmin}, \text{Cmax}, \text{rc}, \text{delr}, \text{augt1}, \text{gsmooth\_factor}, \text{re} \)

where

- \( rc \) = cutoff radius for cutoff function; default = 4.0
- \( delr \) = length of smoothing distance for cutoff function; default = 0.1
- \( \rho_0(I) \) = relative density for element I (overwrites value read from meam file)
- \( Ec(I,J) \) = cohesive energy of reference structure for I-J mixture
- \( \delta(I,J) \) = heat of formation for I-J alloy; if \( Ec_{IJ} \) is input as zero, then LAMMPS sets \( Ec_{IJ} = (Ec_{II} + Ec_{JJ})/2 - \delta_{IJ} \)
- \( \alpha(I,J) \) = alpha parameter for pair potential between I and J (can be computed from bulk modulus of reference structure
- \( re(I,J) \) = equilibrium distance between I and J in the reference structure
- \( C_{max}(I,J,K) \) = Cmax screening parameter when I-J pair is screened by K (I<=J); default = 2.8
- \( C_{min}(I,J,K) \) = Cmin screening parameter when I-J pair is screened by K (I<=J); default = 2.0
- \( \text{lattice}(I,J) \) = lattice structure of I-J reference structure:
  - \( \text{dia} \) = diamond (interlaced fcc for alloy)
  - \( \text{fcc} \) = face centered cubic
  - \( \text{bcc} \) = body centered cubic
  - \( \text{dim} \) = dimer
  - \( \text{b1} \) = rock salt (NaCl structure)
  - \( \text{hcp} \) = hexagonal close-packed
  - \( \text{cl1} \) = MoSi2 structure
  - \( \text{l12} \) = Cu3Au structure (lower case L, followed by 12)
  - \( \text{b2} \) = CsCl structure (interpenetrating simple cubic)
- \( \text{nn2}(I,J) \) = turn on second-nearest neighbor MEAM formulation for I-J pair (see for example (Lee)).
  - 0 = second-nearest neighbor formulation off
  - 1 = second-nearest neighbor formulation on
  - default = 0
- \( \text{attrac}(I,J) \) = additional cubic attraction term in Rose energy I-J pair potential
  - default = 0
- \( \text{repuls}(I,J) \) = additional cubic repulsive term in Rose energy I-J pair potential
  - default = 0
- \( \text{zbl}(I,J) \) = blend the MEAM I-J pair potential with the ZBL potential for small atom separations (ZBL)
  - default = 1
gsMOOTH_factor  = factor determining the length of the G-function smoothing region; only significant for ibar=0 or ibar=4.
   99.0 = short smoothing region, sharp step
   0.5  = long smoothing region, smooth step
default = 99.0
auGt1           = integer flag for whether to augment t1 parameter by 3/5*t3 to account for old vs. new meam formulations.
   0 = don't augment t1
   1 = augment t1
default = 1
ialloy          = integer flag to use alternative averaging rule for t parameters, for comparison with the DYNAMO MEAM code
   0 = standard averaging (matches ialloy=0 in DYNAMO)
   1 = alternative averaging (matches ialloy=1 in DYNAMO)
   2 = no averaging of t (use single-element values)
default = 0
mixture_ref_t   = integer flag to use mixture average of t to compute the background reference density for alloys, instead of the single-element values (see description and warning elsewhere in this doc page)
   0 = do not use mixture averaging for t in the reference density
   1 = use mixture averaging for t in the reference density
default = 0
erose_form      = integer value to select the form of the Rose energy function (see description below).
   default = 0
emb_lin_neg     = integer value to select embedding function for negative densities
   0 = F(rho)=0
   1 = F(rho) = -asub*esub*rho (linear in rho, matches DYNAMO)
default = 0
bkgd_dyn        = integer value to select background density formula
   0 = rho_bkgd = rho_ref_meam(a) (as in the reference structure)
   1 = rho_bkgd = rho0_meam(a)*Z_meam(a) (matches DYNAMO)
default = 0

Rc, delr, re are in distance units (Angstroms in the case of metal units). Ec and delta are in energy units (eV in the case of metal units).

Each keyword represents a quantity which is either a scalar, vector, 2d array, or 3d array and must be specified with the correct corresponding array syntax. The indices I,J,K each run from 1 to N where N is the number of MEAM elements being used.

Thus these lines

rho0(2) = 2.25
alpha(1,2) = 4.37

set rho0 for the 2nd element to the value 2.25 and set alpha for the alloy interaction between elements 1 and 2 to 4.37.

The augt1 parameter is related to modifications in the MEAM formulation of the partial electron density function. In recent literature, an extra term is included in the expression for the third-order density in order to make the densities orthogonal (see for example (Wang), equation 3d); this term is included in the MEAM implementation in lammps. However, in earlier published work this term was not included when deriving parameters, including most of those provided in the library.meam file included with lammps, and to account for this difference the parameter t1 must be augmented by 3/5*t3. If augt1=1, the default, this augmentation is done automatically. When parameter values are fit using the modified density function, as in more recent literature, augt1 should be set to 0.
The mixture_ref_t parameter is available to match results with those of previous versions of lammps (before January 2011). Newer versions of lammps, by default, use the single-element values of the t parameters to compute the background reference density. This is the proper way to compute these parameters. Earlier versions of lammps used an alloy mixture averaged value of t to compute the background reference density. Setting mixture_ref_t=1 gives the old behavior. WARNING: using mixture_ref_t=1 will give results that are demonstrably incorrect for second-neighbor MEAM, and non-standard for first-neighbor MEAM; this option is included only for matching with previous versions of lammps and should be avoided if possible.

The parameters attrac and repuls, along with the integer selection parameter erose_form, can be used to modify the Rose energy function used to compute the pair potential. This function gives the energy of the reference state as a function of interatomic spacing. The form of this function is:

\[
\begin{align*}
astar &= \alpha \times (r/re - 1.d0) \\
\text{if } \text{erose\_form} = 0: \text{erose} &= -E_c \times (1 + \astar + a3 \times (\astar^3)/(r/re)) \times \exp(-\astar) \\
\text{if } \text{erose\_form} = 1: \text{erose} &= -E_c \times (1 + \astar + (-\text{attrac} + \text{repuls}/r) \times (\astar^3)) \times \exp(-\astar) \\
\text{if } \text{erose\_form} = 2: \text{erose} &= -E_c \times (1 + \astar + a3 \times (\astar^3)) \times \exp(-\astar)
\end{align*}
\]

\(a3 = \text{repuls}, \astar < 0\)
\(a3 = \text{attrac}, \astar >= 0\)

Most published MEAM parameter sets use the default values attrac=repulse=0. Setting repuls=attrac=delta corresponds to the form used in several recent published MEAM parameter sets, such as (Vallone)

NOTE: The default form of the erose expression in LAMMPS was corrected in March 2009. The current version is correct, but may show different behavior compared with earlier versions of lammps with the attrac and/or repuls parameters are non-zero. To obtain the previous default form, use erose_form = 1 (this form does not seem to appear in the literature). An alternative form (see e.g. (Lee2)) is available using erose_form = 2.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS with user-specifiable parameters as described above. You never need to specify a pair_coeff command with I != J arguments for this style.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This style is part of the MEAM package. It is only enabled if LAMMPS was built with that package, which also requires the MEAM library be built and linked with LAMMPS. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style eam, pair_style meam/spline

Default: none

(Gullet) Gullet, Wagner, Slepyo, SANDIA Report 2003-8782 (2003). This report may be accessed on-line via this link.


pair_style meam/spline

pair_style meam/spline/omp

Syntax:

pair_style meam/spline

Examples:

pair_style meam/spline
pair_coeff * * Ti.meam.spline Ti
pair_coeff * * Ti.meam.spline Ti Ti Ti

Description:

The meam/spline style computes pairwise interactions for metals using a variant of modified embedded-atom method (MEAM) potentials (Lenosky). The total energy \( E \) is given by

\[
E = \sum_{ij} \phi(r_{ij}) + \sum_i U(\rho_i),
\]

\[
\rho_i = \sum_j \rho(r_{ij}) + \sum_{jk} \tilde{f}(r_{ij}) f(r_{ik}) g[\cos(\theta_{jik})]
\]

where \( \rho_i \) is the density at atom I, \( \theta_{jik} \) is the angle between atoms J, I, and K centered on atom I. The five functions \( \phi, U, \rho, f, \) and \( g \) are represented by cubic splines.

The cutoffs and the coefficients for these spline functions are listed in a parameter file which is specified by the pair_coeff command. Parameter files for different elements are included in the "potentials" directory of the LAMMPS distribution and have a "meam.spline" file suffix. All of these files are parameterized in terms of LAMMPS metal units.

Note that unlike for other potentials, cutoffs for spline-based MEAM potentials are not set in the pair_style or pair_coeff command; they are specified in the potential files themselves.

Unlike the EAM pair style, which retrieves the atomic mass from the potential file, the spline-based MEAM potentials do not include mass information; thus you need to use the mass command to specify it.

Only a single pair_coeff command is used with the meam/spline style which specifies a potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of spline-based MEAM elements to atom types
As an example, imagine the Ti.meam.spline file has values for Ti. If your LAMMPS simulation has 3 atoms types and they are all to be treated with this potentials, you would use the following pair_coeff command:

```
pair_coeff * * Ti.meam.spline Ti Ti Ti
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The three Ti arguments map LAMMPS atom types 1,2,3 to the Ti element in the potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a meam/spline potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

**IMPORTANT NOTE:** The meam/spline style currently supports only single-element MEAM potentials. It may be extended for alloy systems in the future.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

The current version of this pair style does not support multiple element types or mixing. It has been designed for pure elements only.

This pair style does not support the `pair_modify` shift, table, and tail options.

The meam/spline pair style does not write its information to binary restart files, since it is stored in an external potential parameter file. Thus, you need to re-specify the `pair_style` and `pair_coeff` commands in an input script that reads a restart file.

The meam/spline pair style can only be used via the `pair` keyword of the `run_style respa` command. They do not support the `inner`, `middle`, `outer` keywords.

**Restrictions:**

This pair style requires the `newton` setting to be "on" for pair interactions.

This pair style is only enabled if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info.

**Related commands:**

`pair_coeff`, `pair_style meam`
pair_modify command

Syntax:

pair_modify keyword value ...

- one or more keyword/value pairs may be listed
- keyword = shift or mix or table or tabinner or tail or compute

mix value = geometric or arithmetic or sixthpower
shift value = yes or no
table value = N
  2^N = # of values in table	tabinner value = cutoff
cutoff = inner cutoff at which to begin table (distance units)
tail value = yes or no
compute value = yes or no

Examples:

pair_modify shift yes mix geometric
pair_modify tail yes
pair_modify table 12

Description:

Modify the parameters of the currently defined pair style. Not all parameters are relevant to all pair styles.

The mix keyword affects pair coefficients for interactions between atoms of type I and J, when I != J and the coefficients are not explicitly set in the input script. Note that coefficients for I = J must be set explicitly, either in the input script via the "pair_coeff" command or in the "Pair Coeffs" section of the data file. For some pair styles it is not necessary to specify coefficients when I != J, since a "mixing" rule will create them from the I,I and J,J settings. The pair_modify mix value determines what formulas are used to compute the mixed coefficients. In each case, the cutoff distance is mixed the same way as sigma.

Note that not all pair styles support mixing. Also, some mix options are not available for certain pair styles. See the doc page for individual pair styles for those restrictions. Note also that the pair_coeff command also can be to directly set coefficients for a specific I != J pairing, in which case no mixing is performed.

mix geometric

epsilon_ij = sqrt(epsilon_i * epsilon_j)
sigma_ij = sqrt(sigma_i * sigma_j)

mix arithmetic

epsilon_ij = sqrt(epsilon_i * epsilon_j)
sigma_ij = (sigma_i + sigma_j) / 2

mix sixthpower

epsilon_ij = (2 * sqrt(epsilon_i*epsilon_j) * sigma_i^3 * sigma_j^3) / (sigma_i^6 + sigma_j^6)
sigma_ij = ((sigma_i**6 + sigma_j**6) / 2) ^ (1/6)
The *shift* keyword determines whether a Lennard-Jones potential is shifted at its cutoff to 0.0. If so, this adds an energy term to each pairwise interaction which will be included in the thermodynamic output, but does not affect pair forces or atom trajectories. See the doc page for individual pair styles to see which ones support this option.

The *table* keyword applies to pair styles with a long-range Coulombic term; see the doc page for individual styles to see which potentials support this option. If N is non-zero, a table of length $2^N$ is pre-computed for forces and energies, which can shrink their computational cost by up to a factor of 2. The table is indexed via a bit-mapping technique (*Wolff*) and a linear interpolation is performed between adjacent table values. In our experiments with different table styles (lookup, linear, spline), this method typically gave the best performance in terms of speed and accuracy.

The choice of table length is a tradeoff in accuracy versus speed. A larger N yields more accurate force computations, but requires more memory which can slow down the computation due to cache misses. A reasonable value of N is between 8 and 16. The default value of 12 (table of length 4096) gives approximately the same accuracy as the no-table (N = 0) option. For N = 0, forces and energies are computed directly, using a polynomial fit for the needed erfc() function evaluation, which is what earlier versions of LAMMPS did. Values greater than 16 typically slow down the simulation and will not improve accuracy; values from 1 to 8 give unreliable results.

The *tabinner* keyword sets an inner cutoff above which the pairwise computation is done by table lookup (if tables are invoked). The smaller this value is set, the less accurate the table becomes (for a given number of table values), which can require use of larger tables. The default cutoff value is \( \sqrt{2.0} \) distance units which means nearly all pairwise interactions are computed via table lookup for simulations with "real" units, but some close pairs may be computed directly (non-table) for simulations with "lj" units.

When the *tail* keyword is set to *yes*, certain pair styles will add a long-range VanderWaals tail "correction" to the energy and pressure. See the doc page for individual styles to see which support this option. These corrections are included in the calculation and printing of thermodynamic quantities (see the *thermo_style* command). Their effect will also be included in constant NPT or NPH simulations where the pressure influences the simulation box dimensions (e.g. the *fix npt* and *fix nph* commands). The formulas used for the long-range corrections come from equation 5 of (*Sun*).

Several assumptions are inherent in using tail corrections, including the following:

- The simulated system is a 3d bulk homogeneous liquid. This option should not be used for systems that are non-liquid, 2d, have a slab geometry (only 2d periodic), or inhomogeneous.
- \( G(r) \), the radial distribution function (rdf), is unity beyond the cutoff, so a fairly large cutoff should be used (i.e. 2.5 sigma for an LJ fluid), and it is probably a good idea to verify this assumption by checking the rdf. The rdf is not exactly unity beyond the cutoff for each pair of interaction types, so the tail correction is necessarily an approximation.
- Thermophysical properties obtained from calculations with this option enabled will not be thermodynamically consistent with the truncated force-field that was used. In other words, atoms do not feel any LJ pair interactions beyond the cutoff, but the energy and pressure reported by the simulation include an estimated contribution from those interactions.

The *compute* keyword allows pairwise computations to be turned off, even though a *pair_style* is defined. This is not useful for running a real simulation, but can be useful for debugging purposes or for computing only partial forces that do not include the pairwise contribution. You can also do this by simply not defining a *pair_style*, but a Kspace-compatible pair_style is required if you also want to define a *kspace_style*. This keyword gives you that option.

**Restrictions:** none
You cannot use \textit{shift yes} with \textit{tail yes}, since those are conflicting options. You cannot use \textit{tail yes} with 2d simulations.

\textbf{Related commands:}

\texttt{pair\_style, pair\_coeff, thermo\_style}

\textbf{Default:}

The option defaults are mix = geometric, shift = no, table = 12, tabinner = \texttt{sqrt(2.0)}, tail = no, and compute = yes.

Note that some pair styles perform mixing, but only a certain style of mixing. See the doc pages for individual pair styles for details.


pair_style morse command

pair_style morse/cuda command

pair_style morse/gpu command

pair_style morse/omp command

pair_style morse/opt command

Syntax:

pair_style morse cutoff

- cutoff = global cutoff for Morse interactions (distance units)

Examples:

pair_style morse 2.5
pair_coeff * * 100.0 2.0 1.5
pair_coeff 1 1 100.0 2.0 1.5 3.0

Description:

Style morse computes pairwise interactions with the formula

\[ E = D_0 \left[ e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right] \quad r < r_c \]

Rc is the cutoff.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- D0 (energy units)
- alpha (1/distance units)
- r0 (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global morse cutoff is used.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.
These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

None of these pair styles support mixing. Thus, coefficients for all IJ pairs must be specified explicitly.

All of these pair styles support the pair modify shift option for the energy of the pair interaction.

The pair modify table options is not relevant for the Morse pair styles.

None of these pair styles support the pair modify tail option for adding long-range tail corrections to energy and pressure.

All of these pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the pair keyword of the run_style respa command. They do not support the inner, middle, outer keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none
pair_style none command

Syntax:

pair_style none

Examples:

pair_style none

Description:

Using a pair style of none means pair forces are not computed.

With this choice, the force cutoff is 0.0, which means that only atoms within the neighbor skin distance (see the neighbor command) are communicated between processors. You must insure the skin distance is large enough to acquire atoms needed for computing bonds, angles, etc.

A pair style of none will also prevent pairwise neighbor lists from being built. However if the neighbor style is bin, data structures for binning are still allocated. If the neighbor skin distance is small, then these data structures can consume a large amount of memory. So you should either set the neighbor style to nsq or set the skin distance to a larger value.

Restrictions: none

Related commands: none

Default: none
pair_style peri/pmb command

pair_style peri/pmb/omp command

discontinued

pair_style peri/lps command

pair_style peri/lps/omp command

Syntax:

pair_style style

  • style = peri/pmb or peri/lps

Examples:

pair_style peri/pmb
pair_coeff * * 1.6863e22 0.0015001 0.0005 0.25

pair_style peri/lps
pair_coeff * * 14.9e9 14.9e9 0.0015001 0.0005 0.25

Description:

The peridynamic pair styles implement material models that can be used at the microscopic and macroscopic scales.

Style peri/pmb implements the Peridynamic bond-based prototype microelastic brittle (PMB) model.

Style peri/lps implements the Peridynamic state-based linear peridynamic solid (LPS) model.

The canonical papers on Peridynamics are (Silling 2000) and (Silling 2007). The implementation of Peridynamics in LAMMPS is described in (Parks). Also see the PDLAMMPS user guide for more details about the implementation of peridynamics in LAMMPS.

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below.

For the peri/pmb style:

  • c (energy/distance/volume^2 units)
  • horizon (distance units)
  • s00 (unitless)
  • alpha (unitless)

C is the effectively a spring constant for Peridynamic bonds, the horizon is a cutoff distance for truncating interactions, and s00 and alpha are used as a bond breaking criteria. The units of c are such that c/distance = stiffness/volume^2, where stiffness is energy/distance^2 and volume is distance^3. See the users guide for more details.
For the *peri/lps* style:

- \( K \) (force/area units)
- \( G \) (force/area units)
- horizon (distance units)
- \( s_{00} \) (unitless)
- alpha (unitless)

\( K \) is the bulk modulus and \( G \) is the shear modulus. The horizon is a cutoff distance for truncating interactions, and \( s_{00} \) and alpha are used as a bond breaking criteria. See the users guide for more details.

Styles with a *cuda*, *gpu*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These pair styles do not support the pair_modify shift option.

The pair_modify table and tail options are not relevant for these pair styles.

These pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the pair keyword of the run_style respa command. They do not support the inner, middle, outer keywords.

**Restrictions:**

The *peri/pmb* and *peri/lps* styles are part of the PERI package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

pair_coeff

Default: none


pair_style reax command

Syntax:

pair_style reax hbcut hbnewflag tripflag precision

- **hbcut** = hydrogen-bond cutoff (optional) (distance units)
- **hbnewflag** = use old or new hbond function style (0 or 1) (optional)
- **tripflag** = apply stabilization to all triple bonds (0 or 1) (optional)
- **precision** = precision for charge equilibration (optional)

Examples:

pair_style reax
pair_style reax 10.0 0 1 1.0e-5
pair_coeff * * ffield.reax 3 1 2 2
pair_coeff * * ffield.reax 3 NULL NULL 3

Description:

Style *reax* computes the ReaxFF potential of van Duin, Goddard and co-workers. ReaxFF uses distance-dependent bond-order functions to represent the contributions of chemical bonding to the potential energy. There is more than one version of ReaxFF. The version implemented in LAMMPS uses the functional forms documented in the supplemental information of the following paper: (Chenoweth). The version integrated into LAMMPS matches the most up-to-date version of ReaxFF as of summer 2010.

The *reax* style differs from the pair_style reax/c command in the lo-level implementation details. The *reax* style is a Fortran library, linked to LAMMPS. The *reax/c* style was initially implemented as stand-alone C code and is now integrated into LAMMPS as a package.

LAMMPS requires that a file called ffield.reax be provided, containing the ReaxFF parameters for each atom type, bond type, etc. The format is identical to the ffield file used by van Duin and co-workers. The filename is required as an argument in the pair_coeff command. Any value other than "ffield.reax" will be rejected (see below).

LAMMPS provides several different versions of ffield.reax in its potentials dir, each called potentials/ffield.reax.label. These are documented in potentials/README.reax. The default ffield.reax contains parameterizations for the following elements: C, H, O, N, S.

IMPORTANT NOTE: We do not distribute a wide variety of ReaxFF force field files with LAMMPS. Adri van Duin's group at PSU is the central repository for this kind of data as they are continuously deriving and updating parameterizations for different classes of materials. You can visit their WWW site at http://www.engr.psu.edu/adri, register as a "new user", and then submit a request to their group describing material(s) you are interested in modeling with ReaxFF. They can tell you what is currently available or what it would take to create a suitable ReaxFF parameterization.

The format of these files is identical to that used originally by van Duin. We have tested the accuracy of pair_style reax potential against the original ReaxFF code for the systems mentioned above. You can use other ffield files for specific chemical systems that may be available elsewhere (but note that their accuracy may not have been tested).
The *hbcut*, *hbnewflag*, *tripflag*, and *precision* settings are optional arguments. If none are provided, default settings are used: *hbcut* = 6 (which is Angstroms in real units), *hbnewflag* = 1 (use new hbond function style), *tripflag* = 1 (apply stabilization to all triple bonds), and *precision* = 1.0e-6 (one part in 10^6). If you wish to override any of these defaults, then all of the settings must be specified.

Two examples using *pair_style reax* are provided in the examples/reax sub-directory, along with corresponding examples for *pair_style reax/c*.

Use of this pair style requires that a charge be defined for every atom since the *reax* pair style performs a charge equilibration (QEq) calculation. See the *atom_style* and *read_data* commands for details on how to specify charges.

The thermo variable *evdwl* stores the sum of all the ReaxFF potential energy contributions, with the exception of the Coulombic and charge equilibration contributions which are stored in the thermo variable *ecoul*. The output of these quantities is controlled by the *thermo* command.

This pair style tallies a breakdown of the total ReaxFF potential energy into sub-categories, which can be accessed via the *compute pair* command as a vector of values of length 14. The 14 values correspond to the following sub-categories (the variable names in italics match those used in the ReaxFF FORTRAN library):

1. *eb* = bond energy
2. *ea* = atom energy
3. *elp* = lone-pair energy
4. *emol* = molecule energy (always 0.0)
5. *ev* = valence angle energy
6. *epen* = double-bond valence angle penalty
7. *ecoa* = valence angle conjugation energy
8. *ehb* = hydrogen bond energy
9. *et* = torsion energy
10. *eco* = conjugation energy
11. *ew* = van der Waals energy
12. *ep* = Coulomb energy
13. *efi* = electric field energy (always 0.0)
14. *eqeq* = charge equilibration energy

To print these quantities to the log file (with descriptive column headings) the following commands could be included in an input script:

```plaintext
compute reax all pair reax
variable eb     equal c_reax[1]
variable ea     equal c_reax[2]
... variable eqeq equal c_reax[14]
thermo_style custom step temp epair v_eb v_ea ... v_eqeq
```

Only a single *pair_coeff* command is used with the *reax* style which specifies a ReaxFF potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the *pair_coeff* command, where N is the number of LAMMPS atom types:

- *filename*
- *N indices* = mapping of ReaxFF elements to atom types

The specification of the filename and the mapping of LAMMPS atom types recognized by the ReaxFF is done
differently than for other LAMMPS potentials, due to the non-portable difficulty of passing character strings (e.g. filename, element names) between C++ and Fortran.

The filename has to be "ffield.reax" and it has to exist in the directory you are running LAMMPS in. This means you cannot prepend a path to the file in the potentials dir. Rather, you should copy that file into the directory you are running from. If you wish to use another ReaxFF potential file, then name it "ffield.reax" and put it in the directory you run from.

In the ReaxFF potential file, near the top, after the general parameters, is the atomic parameters section that contains element names, each with a couple dozen numeric parameters. If there are M elements specified in the ffield file, think of these as numbered 1 to M. Each of the N indices you specify for the N atom types of LAMMPS atoms must be an integer from 1 to M. Atoms with LAMMPS type 1 will be mapped to whatever element you specify as the first index value, etc. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a ReaxFF potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

IMPORTANT NOTE: Currently the reax pair style cannot be used as part of the hybrid pair style. Some additional changes still need to be made to enable this.

As an example, say your LAMMPS simulation has 4 atom types and the elements are ordered as C, H, O, N in the ffield file. If you want the LAMMPS atom type 1 and 2 to be C, type 3 to be N, and type 4 to be H, you would use the following pair_coeff command:

```
pair_coeff * * ffield.reax 1 1 4 2
```

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

The ReaxFF potential files provided with LAMMPS in the potentials directory are parameterized for real units. You can use the ReaxFF potential with any LAMMPS units, but you would need to create your own potential file with coefficients listed in the appropriate units if your simulation doesn't use "real" units.

Related commands:

```
pair_coeff, pair_style reax/c, fix_reax_bonds
```

Default:

The keyword defaults are hbcut = 6, hbnewflag = 1, tripflag = 1, precision = 1.0e-6.

pair_style reax/c command

Syntax:

pair_style reax/c cfile keyword value

- cfile = NULL or name of a control file
- zero or more keyword/value pairs may be appended

keyword = checkqeq or lgvdw or safezone or mincap
checkqeq value = yes or no = whether or not to require qeq/reax fix
lgvdw value = yes or no = whether or not to use a low gradient vdW correction
safezone = factor used for array allocation
mincap = minimum size for array allocation

Examples:

pair_style reax/c NULL
pair_style reax/c controlfile checkqeq no
pair_style reax/c NULL lgvdw yes
pair_style reax/c NULL safezone 1.6 mincap 100
pair_coeff * * ffield.reax 1 2 2 3

Description:

Style reax/c computes the ReaxFF potential of van Duin, Goddard and co-workers. ReaxFF uses distance-dependent bond-order functions to represent the contributions of chemical bonding to the potential energy. There is more than one version of ReaxFF. The version implemented in LAMMPS uses the functional forms documented in the supplemental information of the following paper: (Chenoweth et al., 2008). The version integrated into LAMMPS matches the most up-to-date version of ReaxFF as of summer 2010. For more technical details about the pair reax/c implementation of ReaxFF, see the (Aktulga) paper.

The reax/c style differs from the pair_style reax command in the lo-level implementation details. The reax style is a Fortran library, linked to LAMMPS. The reax/c style was initially implemented as stand-alone C code and is now integrated into LAMMPS as a package.

LAMMPS provides several different versions of ffield.reax in its potentials dir, each called potentials/ffield.reax.label. These are documented in potentials/README.reax. The default ffield.reax contains parameterizations for the following elements: C, H, O, N, S.

The format of these files is identical to that used originally by van Duin. We have tested the accuracy of pair_style reax/c potential against the original ReaxFF code for the systems mentioned above. You can use other ffield files for specific chemical systems that may be available elsewhere (but note that their accuracy may not have been tested).

IMPORTANT NOTE: We do not distribute a wide variety of ReaxFF force field files with LAMMPS. Adri van Duin's group at PSU is the central repository for this kind of data as they are continuously deriving and updating parameterizations for different classes of materials. You can visit their WWW site at http://www.engr.psu.edu/adri, register as a "new user", and then submit a request to their group describing material(s) you are interested in modeling with ReaxFF. They can tell you what is currently available or what it would take to create a suitable ReaxFF parameterization.
The `cfile` setting can be specified as NULL, in which case default settings are used. A control file can be specified which defines values of control variables. Some control variables are global parameters for the ReaxFF potential. Others define certain performance and output settings. Each line in the control file specifies the value for a control variable. The format of the control file is described below.

IMPORTANT NOTE: The LAMMPS default values for the ReaxFF global parameters correspond to those used by Adri van Duin's stand-alone serial code. If these are changed by setting control variables in the control file, the results from LAMMPS and the serial code will not agree.

Two examples using `pair_style reax/c` are provided in the examples/reax sub-directory, along with corresponding examples for `pair_style reax`.

Use of this pair style requires that a charge be defined for every atom. See the `atom_style` and `read_data` commands for details on how to specify charges.

The ReaxFF parameter files provided were created using a charge equilibration (QEq) model for handling the electrostatic interactions. Therefore, by default, LAMMPS requires that the `fix qeq/reax` command be used with `pair_style reax/c` when simulating a ReaxFF model, to equilibrate charge each timestep. Using the keyword `checkqeq` with the value `no` turns off the check for `fix qeq/reax`, allowing a simulation to be run without charge equilibration. In this case, the static charges you assign to each atom will be used for computing the electrostatic interactions in the system. See the `fix qeq/reax` command for details.

Using the optional keyword `lgvdw` with the value `yes` turns on the low-gradient correction of the ReaxFF/C for long-range London Dispersion, as described in the (Liu) paper. Force field file `ffield.reax.lg` is designed for this correction, and is trained for several energetic materials (see "Liu"). When using lg-correction, recommended value for parameter `thb` is 0.01, which can be set in the control file. Note: Force field files are different for the original or lg corrected pair styles, using wrong ffield file generates an error message.

Optional keywords `safezone` and `mincap` are used for allocating reax/c arrays. Increase these values can avoid memory problems, such as segmentation faults and bondchk failed errors, that could occur under certain conditions.

The thermo variable `evdwl` stores the sum of all the ReaxFF potential energy contributions, with the exception of the Coulombic and charge equilibration contributions which are stored in the thermo variable `ecoul`. The output of these quantities is controlled by the `thermo` command.

This pair style tallies a breakdown of the total ReaxFF potential energy into sub-categories, which can be accessed via the `compute pair` command as a vector of values of length 14. The 14 values correspond to the following sub-categories (the variable names in italics match those used in the original FORTRAN ReaxFF code):

1. `eb` = bond energy
2. `ea` = atom energy
3. `elp` = lone-pair energy
4. `emol` = molecule energy (always 0.0)
5. `ev` = valence angle energy
6. `epen` = double-bond valence angle penalty
7. `ecoa` = valence angle conjugation energy
8. `ehb` = hydrogen bond energy
9. `et` = torsion energy
10. `eco` = conjugation energy
11. `ew` = van der Waals energy
12. `ep` = Coulomb energy
13. efi = electric field energy (always 0.0)
14. eqeq = charge equilibration energy

To print these quantities to the log file (with descriptive column headings) the following commands could be included in an input script:

```plaintext
compute reax all pair reax/c
variable eb      equal c_reax[1]
variable ea      equal c_reax[2]
...
variable eqeq    equal c_reax[14]
thermo_style custom step temp epair v_eb v_ea ... v_eqeq
```

Only a single pair_coeff command is used with the reax/c style which specifies a ReaxFF potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N indices = mapping of ReaxFF elements to atom types

The filename is the ReaxFF potential file. Unlike for the reax pair style, any filename can be used.

In the ReaxFF potential file, near the top, after the general parameters, is the atomic parameters section that contains element names, each with a couple dozen numeric parameters. If there are M elements specified in the ffield file, think of these as numbered 1 to M. Each of the N indices you specify for the N atom types of LAMMPS atoms must be an integer from 1 to M. Atoms with LAMMPS type 1 will be mapped to whatever element you specify as the first index value, etc. If a mapping value is specified as NULL, the mapping is not performed. This can be used when the reax/c style is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

IMPORTANT NOTE: Currently the reax/c pair style cannot be used as part of the hybrid pair style. Some additional work still need to be done to enable this.

As an example, say your LAMMPS simulation has 4 atom types and the elements are ordered as C, H, O, N in the ffield file. If you want the LAMMPS atom type 1 and 2 to be C, type 3 to be N, and type 4 to be H, you would use the following pair_coeff command:

```plaintext
pair_coeff * * ffield.reax 1 1 4 2
```

The format of a line in the control file is as follows:

```plaintext
variable_name value
```
and it may be followed by an "!" character and a trailing comment.

If the value of a control variable is not specified, then default values are used. What follows is the list of variables along with a brief description of their use and default values.

simulation_name: Output files produced by pair_style reax/c carry this name + extensions specific to their contents. Partial energies are reported with a ".pot" extension, while the trajectory file has ".trj" extension.

tabulate_long_range: To improve performance, long range interactions can optionally be tabulated (0 means no tabulation). Value of this variable denotes the size of the long range interaction table. The range from 0 to long range cutoff (defined in the ffield file) is divided into tabulate_long_range points. Then at the start of simulation,
we fill in the entries of the long range interaction table by computing the energies and forces resulting from van der Waals and Coulomb interactions between every possible atom type pairs present in the input system. During the simulation we consult to the long range interaction table to estimate the energy and forces between a pair of atoms. Linear interpolation is used for estimation. (default value = 0)

energy_update_freq: Denotes the frequency (in number of steps) of writes into the partial energies file. (default value = 0)

nbrhood_cutoff: Denotes the near neighbors cutoff (in Angstroms) regarding the bonded interactions. (default value = 5.0)

hbond_cutoff: Denotes the cutoff distance (in Angstroms) for hydrogen bond interactions.(default value = 7.5. Value of 0.0 turns off hydrogen bonds)

bond_graph_cutoff: is the threshold used in determining what is a physical bond, what is not. Bonds and angles reported in the trajectory file rely on this cutoff. (default value = 0.3)

thb_cutoff: cutoff value for the strength of bonds to be considered in three body interactions. (default value = 0.001)

thb_cutoff_sq: cutoff value for the strength of bond order products to be considered in three body interactions. (default value = 0.00001)

write_freq: Frequency of writes into the trajectory file. (default value = 0)

traj_title: Title of the trajectory - not the name of the trajectory file.

atom_info: 1 means print only atomic positions + charge (default = 0)

atom_forces: 1 adds net forces to atom lines in the trajectory file (default = 0)

atom_velocities: 1 adds atomic velocities to atoms line (default = 0)

bond_info: 1 prints bonds in the trajectory file (default = 0)

angle_info: 1 prints angles in the trajectory file (default = 0)

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This pair style is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.
The ReaxFF potential files provided with LAMMPS in the potentials directory are parameterized for real units. You can use the ReaxFF potential with any LAMMPS units, but you would need to create your own potential file with coefficients listed in the appropriate units if your simulation doesn't use "real" units.

**Related commands:**

pair_coeff, fix_qeq_reax, pair_style reax

**Default:**

The keyword defaults are checkqeq = yes, lgvdw = no, safezone = 1.2, mincap = 50.


pair_style resquared command

pair_style resquared/gpu command

pair_style resquared/omp command

Syntax:

pair_style resquared cutoff

  • cutoff = global cutoff for interactions (distance units)

Examples:

pair_style resquared 10.0
pair_coeff * * 1.0 1.0 1.7 3.4 3.4 1.0 1.0 1.0

Description:

Style resquared computes the RE-squared anisotropic interaction (Everaers), (Babadi) between pairs of ellipsoidal and/or spherical Lennard-Jones particles. For ellipsoidal interactions, the potential considers the ellipsoid as being comprised of small spheres of size sigma. LJ particles are a single sphere of size sigma. The distinction is made to allow the pair style to make efficient calculations of ellipsoid/solvent interactions.

Details for the equations used are given in the references below and in this supplementary document.

Use of this pair style requires the NVE, NVT, or NPT fixes with the asphere extension (e.g. fix nve/asphere) in order to integrate particle rotation. Additionally, atom_style ellipsoid should be used since it defines the rotational state and the size and shape of each ellipsoidal particle.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

  • A12 = Energy Prefactor/Hamaker constant (energy units)
  • sigma = atomic interaction diameter (distance units)
  • epsilon_i_a = relative well depth of type I for side-to-side interactions
  • epsilon_i_b = relative well depth of type I for face-to-face interactions
  • epsilon_i_c = relative well depth of type I for end-to-end interactions
  • epsilon_j_a = relative well depth of type J for side-to-side interactions
  • epsilon_j_b = relative well depth of type J for face-to-face interactions
  • epsilon_j_c = relative well depth of type J for end-to-end interactions
  • cutoff (distance units)

The parameters used depend on the type of the interacting particles, i.e. ellipsoids or LJ spheres. The type of a particle is determined by the diameters specified for its 3 shape parameters. If all 3 shape parameters = 0.0, then the particle is treated as an LJ sphere. The epsilon_i_* or epsilon_j_* parameters are ignored for LJ spheres. If the 3 shape parameters are > 0.0, then the particle is treated as an ellipsoid (even if the 3 parameters are equal to each other).

A12 specifies the energy prefactor which depends on the types of the two interacting particles.
For ellipsoid/ellipsoid interactions, the interaction is computed by the formulas in the supplementary document referenced above. $A_{12}$ is the Hamaker constant as described in (Everaers). In LJ units:

$$A_{12} = 4\pi^2 \epsilon_{LJ} (\rho \sigma^3)^2$$

where rho gives the number density of the spherical particles composing the ellipsoids and epsilon_LJ determines the interaction strength of the spherical particles.

For ellipsoid/LJ sphere interactions, the interaction is also computed by the formulas in the supplementary document referenced above. $A_{12}$ has a modified form (see here for details):

$$A_{12} = 4\pi^2 \epsilon_{LJ} (\rho \sigma^3)$$

For ellipsoid/LJ sphere interactions, a correction to the distance-of-closest approach equation has been implemented to reduce the error from two particles of disparate sizes; see this supplementary document.

For LJ sphere/LJ sphere interactions, the interaction is computed using the standard Lennard-Jones formula, which is much cheaper to compute than the ellipsoidal formulas. $A_{12}$ is used as epsilon in the standard LJ formula:

$$A_{12} = \epsilon_{LJ}$$

and the specified sigma is used as the sigma in the standard LJ formula.

When one of both of the interacting particles are ellipsoids, then sigma specifies the diameter of the continuous distribution of constituent particles within each ellipsoid used to model the RE-squared potential. Note that this is a different meaning for sigma than the pair_style gayberne potential uses.

The epsilon_i and epsilon_j coefficients are defined for atom types, not for pairs of atom types. Thus, in a series of pair_coeff commands, they only need to be specified once for each atom type.

Specifically, if any of epsilon_i_a, epsilon_i_b, epsilon_i_c are non-zero, the three values are assigned to atom type I. If all the epsilon_i values are zero, they are ignored. If any of epsilon_j_a, epsilon_j_b, epsilon_j_c are non-zero, the three values are assigned to atom type J. If all three epsilon_i values are zero, they are ignored. Thus the typical way to define the epsilon_i and epsilon_j coefficients is to list their values in "pair_coeff I J" commands when I = J, but set them to 0.0 when I \(!= J. If you do list them when I \(!= J, you should insure they are consistent with their values in other pair_coeff commands.

Note that if this potential is being used as a sub-style of pair_style hybrid, and there is no "pair_coeff I I" setting made for RE-squared for a particular type I (because I-I interactions are computed by another hybrid pair potential), then you still need to insure the epsilon a,b,c coefficients are assigned to that type in a "pair_coeff I J" command.
For large uniform molecules it has been shown that the epsilon energy parameters are approximately representable in terms of local contact curvatures (Everaers):

\[
e_a = \sigma \cdot \frac{a}{b \cdot c}; \quad e_b = \sigma \cdot \frac{b}{a \cdot c}; \quad e_c = \sigma \cdot \frac{c}{a \cdot b}
\]

where \(a, b,\) and \(c\) give the particle diameters.

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used.

Styles with a \texttt{cuda}, \texttt{gpu}, \texttt{omp}, or \texttt{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \texttt{-suffix} command-line switch when you invoke LAMMPS, or you can use the \texttt{suffix} command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.


text1

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs \(I,J\) and \(I \neq J\), the epsilon and sigma coefficients and cutoff distance can be mixed, but only for sphere pairs. The default mix value is geometric. See the "pair_modify" command for details. Other type pairs cannot be mixed, due to the different meanings of the energy prefactors used to calculate the interactions and the implicit dependence of the ellipsoid-sphere interaction on the equation for the Hamaker constant presented here. Mixing of sigma and epsilon followed by calculation of the energy prefactors using the equations above is recommended.

This pair styles supports the \texttt{pair_modify} shift option for the energy of the Lennard-Jones portion of the pair interaction, but only for sphere-sphere interactions. There is no shifting performed for ellipsoidal interactions due to the anisotropic dependence of the interaction.

The \texttt{pair_modify} table option is not relevant for this pair style.

This pair style does not support the \texttt{pair_modify} tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the \texttt{pair} keyword of the \texttt{run_style respa} command. It does not support the \texttt{inner}, \texttt{middle}, \texttt{outer} keywords of the \texttt{run_style command}. 
Restrictions:

This style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This pair style requires that atoms be ellipsoids as defined by the atom_style ellipsoid command.

Particles acted on by the potential can be extended aspherical or spherical particles, or point particles. Spherical particles have all 3 of their shape parameters equal to each other. Point particles have all 3 of their shape parameters equal to 0.0.

The distance-of-closest-approach approximation used by LAMMPS becomes less accurate when high-aspect ratio ellipsoids are used.

Related commands:

pair_coeff, fix nve/asphere, compute temp/asphere, pair_style gayberne

Default: none


pair_style lj/sdk command

pair_style lj/sdk/gpu command

pair_style lj/sdk/omp command

pair_style lj/sdk/coul/long command

pair_style lj/sdk/coul/long/gpu command

pair_style lj/sdk/coul/long/omp command

Syntax:

pair_style style args

- style = lj/sdk or lj/sdk/coul/long
- args = list of arguments for a particular style

lj/sdk args = cutoff
   cutoff = global cutoff for Lennard Jones interactions (distance units)

lj/sdk/coul/long args = cutoff (cutoff2)
   cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
   cutoff2 = global cutoff for Coulombic (optional) (distance units)

Examples:

pair_style lj/sdk 2.5
pair_coeff 1 1 lj12_6 1 1.1 2.8

pair_style lj/sdk/coul/long 10.0
pair_style lj/sdk/coul/long 10.0 12.0
pair_coeff 1 1 lj9_6 100.0 3.5 12.0

Description:

The *lj/sdk* styles compute a 9/6, 12/4, or 12/6 Lennard-Jones potential, given by

\[
E = \frac{27}{4} \epsilon \left[ \left( \frac{\sigma}{r} \right)^9 - \left( \frac{\sigma}{r} \right)^{6} \right] \quad r < r_c
\]

\[
E = \frac{3\sqrt{3}}{2} \epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{4} \right] \quad r < r_c
\]

\[
E = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right] \quad r < r_c
\]
as required for the SDK Coarse-grained MD parametrization discussed in (Shinoda) and (DeVane). Rc is the
cutoff.

Style *lj/sdk/coul/long* computes the adds Coulombic interactions with an additional damping factor applied so it
can be used in conjunction with the *kspace_style* command and its *ewald* or *pppm* or *pppm/cg* option. The
Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed
directly; interactions outside that distance are computed in reciprocal space.

The following coefficients must be defined for each pair of atoms types via the *pair_coeff* command as in the
examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as
described below:

- cg_type (lj9_6, lj12_4, or lj12_6)
- epsilon (energy units)
- sigma (distance units)
- cutoff1 (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy
minimum. The prefactors are chosen so that the potential minimum is at -epsilon.

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the
pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic
interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for
this type pair.

For *lj/sdk/coul/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an
individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *cuda*, *gpu*, *omp* or *opt* suffix are functionally the same as the corresponding style without the suffix.
They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate
of the manual. The accelerated styles take the same arguments and should produce the same results, except for
round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP, and OPT packages respectively. They
are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the
-suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input
script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, and rRESPA info:**

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/sdk pair
styles *cannot* be mixed, since different pairs may have different exponents. So all parameters for all pairs have to
be specified explicitly through the “pair_coeff” command. Defining then in a data file is also not supported, due to
limitations of that file format.

All of the lj/sdk pair styles support the pair_modify shift option for the energy of the Lennard-Jones portion of the
pair interaction.
The \textit{lj/sdk/coul/long} pair styles support the \texttt{pair_modify} table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

All of the \textit{lj/sdk} pair styles write their information to \texttt{binary restart files}, so \texttt{pair_style} and \texttt{pair_coeff} commands do not need to be specified in an input script that reads a restart file.

The \textit{lj/sdk} and \textit{lj/cut/coul/long} pair styles do not support the use of the \textit{inner}, \textit{middle}, and \textit{outer} keywords of the \texttt{run_style respa} command.

**Restrictions:**

All of the \textit{lj/sdk} pair styles are part of the USER-CG-CMM package. The \textit{lj/sdk/coul/long} style also requires the KSPACE package to be built (which is enabled by default). They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

\texttt{pair_coeff}, \texttt{angle_style sdk}

**Default:** None

(Shinoda) Shinoda, DeVane, Klein, Mol Sim, 33, 27 (2007).

**pair_style soft command**

**pair_style soft/omp command**

Syntax:

```
pair_style soft cutoff
```

- cutoff = global cutoff for soft interactions (distance units)

**Examples:**

```
pair_style soft 2.5
pair_coeff * * 10.0
pair_coeff 1 1 10.0 3.0

pair_style soft 2.5
pair_coeff * * 0.0
variable prefactor equal ramp(0,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

**Description:**

Style *soft* computes pairwise interactions with the formula

\[
E = A \left[ 1 + \cos \left( \frac{\pi r}{r_c} \right) \right] \quad r < r_c
\]

It is useful for pushing apart overlapping atoms, since it does not blow up as r goes to 0. A is a pre-factor that can be made to vary in time from the start to the end of the run (see discussion below), e.g. to start with a very soft potential and slowly harden the interactions over time. Rc is the cutoff. See the *fix nve/limit* command for another way to push apart overlapping atoms.

The following coefficients must be defined for each pair of atom types via the *pair_coeff* command as in the examples above, or in the data file or restart files read by the *read_data* or *read_restart* commands, or by mixing as described below:

- A (energy units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global soft cutoff is used.

**IMPORTANT NOTE:** The syntax for *pair_coeff* with a single A coeff is different in the current version of LAMMPS than in older versions which took two values, Astart and Astop, to ramp between them. This functionality is now available in a more general form through the *fix adapt* command, as explained below. Note that if you use an old input script and specify Astart and Astop without a cutoff, then LAMMPS will interpret that as A and a cutoff, which is probably not what you want.
The `fix adapt` command can be used to vary A for one or more pair types over the course of a simulation, in which case `pair_coeff` settings for A must still be specified, but will be overridden. For example, these commands will vary the prefactor A for all pairwise interactions from 0.0 at the beginning to 30.0 at the end of a run:

```plaintext
variable prefactor equal ramp(0,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

Note that a formula defined by an `equal-style variable` can use the current timestep, elapsed time in the current run, elapsed time since the beginning of a series of runs, as well as access other variables.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is always mixed via a `geometric` rule. The cutoff is mixed according to the `pair_modify mix` value. The default mix value is `geometric`. See the "pair_modify" command for details.

This pair style does not support the `pair_modify` shift option, since the pair interaction goes to 0.0 at the cutoff.

The `pair_modify` table and tail options are not relevant for this pair style.

This pair style writes its information to binary restart files, so `pair_style` and `pair_coeff` commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner`, `middle`, `outer` keywords.

**Restrictions:** none

**Related commands:**

`pair_coeff`, `fix nve/limit`, `fix adapt`

**Default:** none
pair_style sph/heatconduction command

Syntax:

pair_style sph/heatconduction

Examples:

pair_style sph/heatconduction
pair_coeff * * 1.0 2.4

Description:

The sph/heatconduction style computes heat transport between SPH particles. The transport model is the diffusion equation for the internal energy.

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- D diffusion coefficient (length^2/time units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_sph/rhosum

Default: none
pair_style sph/idealgas command

Syntax:

pair_style sph/idealgas

Examples:

pair_style sph/idealgas
pair_coeff * * 1.0 2.4

Description:

The sph/idealgas style computes pressure forces between particles according to the ideal gas equation of state:

\[ p = (\gamma - 1) \rho e \]

where \( \gamma = 1.4 \) is the heat capacity ratio, \( \rho \) is the local density, and \( e \) is the internal energy per unit mass. This pair style also computes Monaghan's artificial viscosity to prevent particles from interpenetrating (Monaghan).

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- \( \nu \) artificial viscosity (no units)
- \( h \) kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:
pair_coeff, pair_sph/rhosum

Default: none

pair_style sph/lj command

Syntax:

pair_style sph/lj

Examples:

pair_style sph/lj
pair_coeff * * 1.0 2.4

Description:

The sph/lj style computes pressure forces between particles according to the Lennard-Jones equation of state, which is computed according to Ree's 1980 polynomial fit (Ree). The Lennard-Jones parameters epsilon and sigma are set to unity. This pair style also computes Monaghan's artificial viscosity to prevent particles from interpenetrating (Monaghan).

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- nu artificial viscosity (no units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

As noted above, the Lennard-Jones parameters epsilon and sigma are set to unity.

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_sph/rhosum

Default: none
(Ree) Ree, Journal of Chemical Physics, 73, 5401 (1980).

**pair_style sph/rhosum command**

**Syntax:**

```
pair_style sph/rhosum Nstep
```

- `Nstep` = timestep interval

**Examples:**

```
pair_style sph/rhosum 10
pair_coeff * * 2.4
```

**Description:**

The sph/rhosum style computes the local particle mass density \( \rho \) for SPH particles by kernel function interpolation, every \( Nstep \) timesteps.

See [this PDF guide](#) to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the `pair_coeff` command as in the examples above.

- `h` (distance units)

**Mixing, shift, table, tail correction, restart, rRESPA info:**

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the `pair_modify` shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner`, `middle`, `outer` keywords.

**Restrictions:**

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the [Making LAMMPS](#) section for more info.

**Related commands:**

`pair_coeff`, `pair_sph/taitwater`

**Default:** none
pair_style sph/taitwater command

Syntax:

pair_style sph/taitwater

Examples:

pair_style sph/taitwater
pair_coeff * * 1000.0 1430.0 1.0 2.4

Description:

The sph/taitwater style computes pressure forces between SPH particles according to Tait's equation of state:

\[ p = B \left[ \left( \frac{\rho}{\rho_0} \right)^\gamma - 1 \right] \]

where \( \gamma = 7 \) and \( B = c_0^2 \rho_0 / \gamma \), with \( \rho_0 \) being the reference density and \( c_0 \) the reference speed of sound.

This pair style also computes Monaghan's artificial viscosity to prevent particles from interpenetrating (Monaghan).

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- \( \rho_0 \) reference density (mass/volume units)
- \( c_0 \) reference soundspeed (distance/time units)
- \( \nu \) artificial viscosity (no units)
- \( h \) kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:
This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_sph/rhosum

Default: none

pair_style sph/taitwater/morris command

Syntax:

```
pair_style sph/taitwater/morris
```

Examples:

```
pair_style sph/taitwater/morris
pair_coeff * * 1000.0 1430.0 1.0 2.4
```

Description:

The sph/taitwater/morris style computes pressure forces between SPH particles according to Tait’s equation of state:

\[
p = B \left[ \left( \frac{\rho}{\rho_0} \right)^\gamma - 1 \right]
\]

where \( \gamma = 7 \) and \( B = c_0^2 \rho_0 / \gamma \), with \( \rho_0 \) being the reference density and \( c_0 \) the reference speed of sound.

This pair style also computes laminar viscosity (Morris).

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the `pair_coeff` command as in the examples above.

- \( \rho_0 \) reference density (mass/volume units)
- \( c_0 \) reference soundspeed (distance/time units)
- \( \nu \) dynamic viscosity (mass*distance/time units)
- \( h \) kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the `pair_modify` shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the `pair_style` and `pair_coeff` commands in an input script that reads a restart file.

This style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner`, `middle`, `outer` keywords.

Restrictions:
This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

**Related commands:**

`pair_coeff`, `pair_sph/rhosum`

**Default:** none

**pair_style command**

**Syntax:**

```
pair_style style args
```

- `style` = one of the styles from the list below
- `args` = arguments used by a particular style

**Examples:**

```
pair_style lj/cut 2.5
pair_style eam/alloy
pair_style hybrid lj/charmm/coul/long 10.0 eam
pair_style table linear 1000
pair_style none
```

**Description:**

Set the formula(s) LAMMPS uses to compute pairwise interactions. In LAMMPS, pair potentials are defined between pairs of atoms that are within a cutoff distance and the set of active interactions typically changes over time. See the **bond_style** command to define potentials between pairs of bonded atoms, which typically remain in place for the duration of a simulation.

In LAMMPS, pairwise force fields encompass a variety of interactions, some of which include many-body effects, e.g. EAM, Stillinger-Weber, Tersoff, REBO potentials. They are still classified as "pairwise" potentials because the set of interacting atoms changes with time (unlike molecular bonds) and thus a neighbor list is used to find nearby interacting atoms.

Hybrid models where specified pairs of atom types interact via different pair potentials can be setup using the **hybrid** pair style.

The coefficients associated with a pair style are typically set for each pair of atom types, and are specified by the **pair_coeff** command or read from a file by the **read_data** or **read_restart** commands.

The **pair_modify** command sets options for mixing of type I-J interaction coefficients and adding energy offsets or tail corrections to Lennard-Jones potentials. Details on these options as they pertain to individual potentials are described on the doc page for the potential. Likewise, info on whether the potential information is stored in a restart file is listed on the potential doc page.

In the formulas listed for each pair style, $E$ is the energy of a pairwise interaction between two atoms separated by a distance $r$. The force between the atoms is the negative derivative of this expression.

If the **pair_style** command has a cutoff argument, it sets global cutoffs for all pairs of atom types. The distance(s) can be smaller or larger than the dimensions of the simulation box.

Typically, the global cutoff value can be overridden for a specific pair of atom types by the **pair_coeff** command. The pair style settings (including global cutoffs) can be changed by a subsequent **pair_style** command using the same style. This will reset the cutoffs for all atom type pairs, including those previously set explicitly by a **pair_coeff** command. The exceptions to this are that **pair_style** **table** and **hybrid** settings cannot be reset. A new **pair_style** command for these styles will wipe out all previously specified **pair_coeff** values.
Here is an alphabetic list of pair styles defined in LAMMPS. Click on the style to display the formula it computes, arguments specified in the pair_style command, and coefficients specified by the associated pair_coeff command.

Note that there are also additional pair styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the pair section of this page.

There are also additional accelerated pair styles included in the LAMMPS distribution for faster performance on CPUs and GPUs. The list of these with links to the individual styles are given in the pair section of this page.

- **pair_style none** - turn off pairwise interactions
- **pair_style hybrid** - multiple styles of pairwise interactions
- **pair_style hybrid/overlay** - multiple styles of superposed pairwise interactions

- **pair_style adp** - angular dependent potential (ADP) of Mishin
- **pair_style airebo** - AIREBO potential of Stuart
- **pair_style bop** - BOP potential of Pettifor
- **pair_style born** - Born-Mayer-Huggins potential
- **pair_style born/coul/long** - Born-Mayer-Huggins with long-range Coulombics
- **pair_style born/coul/wolf** - Born-Mayer-Huggins with Coulombics via Wolf potential
- **pair_style brownian** - Brownian potential for Fast Lubrication Dynamics
- **pair_style brownian/poly** - Brownian potential for Fast Lubrication Dynamics with polydispersity
- **pair_style buck** - Buckingham potential
- **pair_style buck/coul/cut** - Buckingham with cutoff Coulomb
- **pair_style buck/coul/long** - Buckingham with long-range Coulomb
- **pair_style colloid** - integrated colloidal potential
- **pair_style comb** - charge-optimized many-body (COMB) potential
- **pair_style coul/cut** - cutoff Coulombic potential
- **pair_style coul/debye** - cutoff Coulombic potential with Debye screening
- **pair_style coul/long** - long-range Coulombic potential
- **pair_style coul/wolf** - Coulombics via Wolf potential
- **pair_style dipole/cut** - point dipoles with cutoff
- **pair_style dpd** - dissipative particle dynamics (DPD)
- **pair_style dpd/tstat** - DPD thermostatting
- **pair_style dsmc** - Direct Simulation Monte Carlo (DSMC)
- **pair_style eam** - embedded atom method (EAM)
- **pair_style eam/alloy** - alloy EAM
- **pair_style eam/fs** - Finnis-Sinclair EAM
- **pair_style eim** - embedded ion method (EIM)
- **pair_style gauss** - Gaussian potential
- **pair_style gayberne** - Gay-Berne ellipsoidal potential
- **pair_style gran/hertz/history** - granular potential with Hertzian interactions
- **pair_style gran/hooke** - granular potential with history effects
- **pair_style gran/hooke/history** - granular potential without history effects
- **pair_style hbond/dreiding/lj** - DREIDING hydrogen bonding LJ potential
- **pair_style hbond/dreiding/morse** - DREIDING hydrogen bonding Morse potential
- **pair_style lcbop** - long-range bond-order potential (LCBOP)
- **pair_style line/lj** - LJ potential between line segments
- **pair_style lj/charmm/coul/charmm** - CHARMM potential with cutoff Coulomb
- **pair_style lj/charmm/coul/charmm/implicit** - CHARMM for implicit solvent
- **pair_style lj/charmm/coul/long** - CHARMM with long-range Coulomb
- **pair_style lj/class2** - COMPASS (class 2) force field with no Coulomb
- **pair_style lj/class2/coul/cut** - COMPASS with cutoff Coulomb
- **pair_style lj/class2/coul/long** - COMPASS with long-range Coulomb
- **pair_style lj/cut** - cutoff Lennard-Jones potential with no Coulomb
- **pair_style lj/cut/coul/cut** - LJ with cutoff Coulomb
- **pair_style lj/cut/coul/debye** - LJ with Debye screening added to Coulomb
- **pair_style lj/cut/coul/long** - LJ with long-range Coulomb
- **pair_style lj/cut/coul/long/tip4p** - LJ with long-range Coulomb for TIP4P water
- **pair_style lj/cut/coul/long/tip4p** - LJ with long-range Coulomb for TIP4P water
- **pair_style lj/expand** - Lennard-Jones for variable size particles
- **pair_style lj/gromacs** - GROMACS-style Lennard-Jones potential
- **pair_style lj/gromacs/coul/gromacs** - GROMACS-style LJ and Coulombic potential
- **pair_style lj/smooth** - smoothed Lennard-Jones potential
- **pair_style lj/smooth/linear** - linear smoothed Lennard-Jones potential
- **pair_style lj96/cut** - Lennard-Jones 9/6 potential
- **pair_style lubricate** - hydrodynamic lubrication forces
- **pair_style lubricate/poly** - hydrodynamic lubrication forces with polydispersity
- **pair_style lubricateU** - hydrodynamic lubrication forces for Fast Lubrication Dynamics
- **pair_style lubricateU/poly** - hydrodynamic lubrication forces for Fast Lubrication with polydispersity
- **pair_style meam** - modified embedded atom method (MEAM)
- **pair_style morse** - Morse potential
- **pair_style peri/lps** - peridynamic LPS potential
- **pair_style peri/pmb** - peridynamic PMB potential
- **pair_style reax** - ReaxFF potential
- **pair_style rebo** - 2nd generation REBO potential of Brenner
- **pair_style resquared** - Everaers RE-Squared ellipsoidal potential
- **pair_style soft** - Soft (cosine) potential
- **pair_style sw** - Stillinger-Weber 3-body potential
- **pair_style table** - tabulated pair potential
- **pair_style tersoff** - Tersoff 3-body potential
- **pair_style tersoff/zbl** - Tersoff/ZBL 3-body potential
- **pair_style tri/lj** - LJ potential between triangles
- **pair_style yukawa** - Yukawa potential
- **pair_style yukawa/colloid** - screened Yukawa potential for finite-size particles

**Restrictions:**

This command must be used before any coefficients are set by the `pair_coeff`, `read_data`, or `read_restart` commands.

Some pair styles are part of specific packages. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual pair potentials tell if it is part of a package.

**Related commands:**

`pair_coeff`, `read_data`, `pair_modify`, `kspace_style`, `dielectric`, `pair_write`

**Default:**

`pair_style none`
pair_style sw command

pair_style sw/cuda command

pair_style sw/omp command

Syntax:

pair_style sw

Examples:

pair_style sw
pair_coeff * * si.sw Si
pair_coeff * * GaN.sw Ga N Ga

Description:

The sw style computes a 3-body Stillinger-Weber potential for the energy $E$ of a system of atoms as

$$E = \sum_i \sum_j (r_{ij}) + \sum_i \sum_{j \neq i} \sum_k (r_{ij}, r_{ik}, \theta_{ijk})$$

$$\phi_2(r_{ij}) = A_{ij} \epsilon_{ij} \left[ B_{ij} \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{p_{ij}} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{q_{ij}} \right] \exp \left( \frac{\sigma_{ij}}{r_{ij} - a_{ij} \sigma_{ij}} \right)$$

$$\phi_3(r_{ij}, r_{ik}, \theta_{ijk}) = \lambda_{ijk} \epsilon_{ijk} \left[ \cos \theta_{ijk} - \cos \theta_{0ijk} \right] \exp \left( \frac{\gamma_{ij} \sigma_{ij}}{r_{ij} - a_{ij} \sigma_{ij}} \right) \exp \left( \frac{\gamma_{ik} \sigma_{ij}}{r_{ik} - a_{ik} \sigma_{ij}} \right)$$

where $\phi_2$ is a two-body term and $\phi_3$ is a three-body term. The summations in the formula are over all neighbors $J$ and $K$ of atom $I$ within a cutoff distance = $a*sigma$.

Only a single pair_coeff command is used with the sw style which specifies a Stillinger-Weber potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying $N$ additional arguments after the filename in the pair_coeff command, where $N$ is the number of LAMMPS atom types:

- filename
- $N$ element names = mapping of SW elements to atom types

As an example, imagine a file SiC.sw has Stillinger-Weber values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

pair_coeff * * SiC.sw Si Si Si C
The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the SW file. The final C argument maps LAMMPS atom type 4 to the C element in the SW file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a sw potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Stillinger-Weber files in the potentials directory of the LAMMPS distribution have a ".sw" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to the two-body and three-body coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2
- element 3
- epsilon (energy units)
- sigma (distance units)
- a
- lambda
- gamma
- costheta0
- A
- B
- p
- q
- tol

The A, B, p, and q parameters are used only for two-body interactions. The lambda and costheta0 parameters are used only for three-body interactions. The epsilon, sigma, and a parameters are used for both two-body and three-body interactions. gamma is used only in the three-body interactions, but is defined for pairs of atoms. The non-annotated parameters are unitless.

LAMMPS introduces an additional performance-optimization parameter tol that is used for both two-body and three-body interactions. In the Stillinger-Weber potential, the interaction energies become negligibly small at atomic separations substantially less than the theoretical cutoff distances. LAMMPS therefore defines a virtual cutoff distance based on a user defined tolerance tol. The use of the virtual cutoff distance in constructing atom neighbor lists can significantly reduce the neighbor list sizes and therefore the computational cost. LAMMPS provides a tol value for each of the three-body entries so that they can be separately controlled. If tol = 0.0, then the standard Stillinger-Weber cutoff is used.

The Stillinger-Weber potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify SW parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction. Thus an entry for SiCC means a Si atom with 2 C atoms as neighbors. The parameter values used for the two-body interaction come from the entry where the 2nd and 3rd elements are the same. Thus the two-body parameters for Si interacting with C, comes from the SiCC entry. The three-body parameters can in principle be specific to the three elements of the configuration. In the literature, however, the three-body parameters are usually defined by simple formulas.
involving two sets of pair-wise parameters, corresponding to the \(ij\) and \(ik\) pairs, where \(i\) is the center atom. The user must ensure that the correct combining rule is used to calculate the values of the three-body parameters for alloys. Note also that the function \(\phi_3\) contains two exponential screening factors with parameter values from the \(ij\) pair and \(ik\) pairs. So \(\phi_3\) for a C atom bonded to a Si atom and a second C atom will depend on the three-body parameters for the CSiC entry, and also on the two-body parameters for the CCC and CSiSi entries. Since the order of the two neighbors is arbitrary, the threebody parameters for entries CSiC and CCSi should be the same. Similarly, the two-body parameters for entries SiCC and CSiSi should also be the same. The parameters used only for two-body interactions (\(A, B, p,\) and \(q\)) in entries whose 2nd and 3rd element are different (e.g. SiCSi) are not used for anything and can be set to 0.0 if desired. This is also true for the parameters in \(\phi_3\) that are taken from the \(ij\) and \(ik\) pairs (\(\sigma, a, \gamma\))

Styles with a \textit{cuda}, \textit{gpu}, \textit{omp}, or \textit{opt} suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the \textit{-suffix} command-line switch when you invoke LAMMPS, or you can use the \textit{suffix} command in your input script.

See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I \(!= J\), where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the \textit{pair_modify} shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the \textit{pair_style} and \textit{pair_coeff} commands in an input script that reads a restart file.

This pair style can only be used via the \textit{pair} keyword of the \textit{run_style respa} command. It does not support the \textit{inner}, \textit{middle}, \textit{outer} keywords.

Restrictions:

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair style requires the \textit{newton} setting to be "on" for pair interactions.

The Stillinger-Weber potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the SW potential with any LAMMPS units, but you would need to create your own SW potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

\texttt{pair_coeff}
pair_style table command

pair_style table/gpu command

pair_style table/omp command

Syntax:

pair_style table style N

- style = lookup or linear or spline or bitmap = method of interpolation
- N = use N values in lookup, linear, spline tables
- N = use 2^N values in bitmap tables

Examples:

pair_style table linear 1000
pair_style table bitmap 12
pair_coeff * 3 morse.table ENTRY1
pair_coeff * 3 morse.table ENTRY1 7.0

Description:

Style table creates interpolation tables of length N from pair potential and force values listed in a file(s) as a function of distance. The files are read by the pair_coeff command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and force values at each of N distances. During a simulation, these tables are used to interpolate energy and force values as needed. The interpolation is done in one of 4 styles: lookup, linear, spline, or bitmap.

For the lookup style, the distance between 2 atoms is used to find the nearest table entry, which is the energy or force.

For the linear style, the pair distance is used to find 2 surrounding table values from which an energy or force is computed by linear interpolation.

For the spline style, a cubic spline coefficients are computed and stored at each of the N values in the table. The pair distance is used to find the appropriate set of coefficients which are used to evaluate a cubic polynomial which computes the energy or force.

For the bitmap style, the N means to create interpolation tables that are 2^N in length. (Wolff) and a linear interpolation is performed between adjacent table values.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- filename
- keyword
- cutoff (distance units)
The filename specifies a file containing tabulated energy and force values. The keyword specifies a section of the file. The cutoff is an optional coefficient. If not specified, the outer cutoff in the table itself (see below) will be used to build an interpolation table that extend to the largest tabulated distance. If specified, only file values up to the cutoff are used to create the interpolation table. The format of this file is described below.

Here are some guidelines for using the pair_style table command to best effect:

- Vary the number of table points; you may need to use more than you think to get good resolution.
- Always use the pair_write command to produce a plot of what the final interpolated potential looks like. This can show up interpolation "features" you may not like.
- Start with the linear style; it's the style least likely to have problems.
- Use \textit{N} in the pair_style command equal to the "\textit{N}" in the tabulation file, and use the "RSQ" or "BITMAP" parameter, so additional interpolation is not needed. See discussion below.
- Make sure that your tabulated forces and tabulated energies are consistent (dE/dr = -F) along the entire range of \( r \) values.
- Use as large an inner cutoff as possible. This avoids fitting splines to very steep parts of the potential.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# Morse potential for Fe   (one or more comment or blank lines)
MORSE_FE                   (keyword is first text on line)
N 500 R 1.0 10.0           (N, R, RSQ, BITMAP, FPRIME parameters)
(blank)
1 1.0 25.5 102.34          (index, r, energy, force)
2 1.02 23.4 98.5
...
500 10.0 0.001 0.003
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the pair_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "\textit{N}" is required and its value is the number of table entries that follow. Note that this may be different than the \textit{N} specified in the pair_style table command. Let \textit{Ntable} = \textit{N} in the pair_style command, and \textit{Nfile} = "\textit{N}" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the \textit{Nfile} tabulated values as nodal points. It uses these to interpolate as needed to generate energy and force values at \textit{Ntable} different points. The resulting tables of length \textit{Ntable} are then used as described above, when computing energy and force for individual pair distances. This means that if you want the interpolation tables of length \textit{Ntable} to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set \textit{Ntable} = \textit{Nfile}, and use the "RSQ" or "BITMAP" parameter. The internal table abscissa is RSQ (separation distance squared).

All other parameters are optional. If "\textit{R}" or "RSQ" or "BITMAP" does not appear, then the distances in each line of the table are used as-is to perform spline interpolation. In this case, the table values can be spaced in \( r \) uniformly or however you wish to position table values in regions of large gradients.

If used, the parameters "\textit{R}" or "RSQ" are followed by 2 values \textit{rlo} and \textit{rhi}. If specified, the distance associated with each energy and force value is computed from these 2 values (at high accuracy), rather than using the (low-accuracy) value listed in each line of the table. The distance values in the table file are ignored in this case. For "\textit{R}"", distances uniformly spaced between \textit{rlo} and \textit{rhi} are computed; for "RSQ", squared distances uniformly spaced between \textit{rlo}^2\textit{rlo} and \textit{rhi}^2\textit{rhi} are computed.
If used, the parameter "BITMAP" is also followed by 2 values rlo and rhi. These values, along with the "N" value determine the ordering of the N lines that follow and what distance is associated with each. This ordering is complex, so it is not documented here, since this file is typically produced by the pair_write command with its bitmap option. When the table is in BITMAP format, the "N" value in the file must be equal to 2^M where M is the value specified in the pair_style command. Also, a cutoff parameter cannot be used as an optional 3rd argument in the pair_coeff command; the entire table extent as specified in the file must be used.

If used, the parameter "FPRIME" is followed by 2 values fplo and fphi which are the derivative of the force at the innermost and outermost distances listed in the table. These values are needed by the spline construction routines. If not specified by the "FPRIME" parameter, they are estimated (less accurately) by the first 2 and last 2 force values in the table. This parameter is not used by BITMAP tables.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is r (in distance units), the 3rd value is the energy (in energy units), and the 4th is the force (in force units). The r values must increase from one line to the next (unless the BITMAP parameter is specified).

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The pair_modify shift, table, and tail options are not relevant for this pair style.

This pair style writes the settings for the "pair_style table" command to binary restart files, so a pair_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, pair_coeff commands do need to be specified in the restart input script.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions: none

Related commands:

pair_coeff
pair_style tersoff command

pair_style tersoff/table command

pair_style tersoff/cuda

pair_style tersoff/omp

pair_style tersoff/table/omp command

Syntax:

pair_style style

style = tersoff or tersoff/table or tersoff/cuda or tersoff/omp or tersoff/table/omp

Examples:

pair_style tersoff
pair_coeff * * Si.tersoff Si
pair_coeff * * SiC.tersoff Si C Si

pair_style tersoff/table
pair_coeff * * SiCGe.tersoff Si(D)

Description:

The tersoff style computes a 3-body Tersoff potential (Tersoff_1) for the energy E of a system of atoms as
\[ E = \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij} \]

\[ V_{ij} = f_C(r_{ij}) \left[ f_R(r_{ij}) + b_{ij} f_A(r_{ij}) \right] \]

\[ f_C(r) = \begin{cases} 
1 & : r < R - D \\
\frac{1}{2} - \frac{1}{2} \sin \left( \frac{\pi (r - R)}{D} \right) & : R - D < r < R + D \\
0 & : r > R + D 
\end{cases} \]

\[ f_R(r) = A \exp(-\lambda_1 r) \]

\[ f_A(r) = -B \exp(-\lambda_2 r) \]

\[ b_{ij} = (1 + \beta^n \zeta_{ij}^n)^{-\frac{1}{2n}} \]

\[ \zeta_{ij} = \sum_{k \neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp \left[ \lambda_3 m (r_{ij} - r_{ik})^m \right] \]

\[ g(\theta) = \gamma_{ijk} \left( 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (\cos \theta - \cos \theta_0)^2} \right) \]

where \( f_R \) is a two-body term and \( f_A \) includes three-body interactions. The summations in the formula are over all neighbors \( J \) and \( K \) of atom \( I \) within a cutoff distance = \( R + D \).

The \textit{tersoff/table} style uses tabulated forms for the two-body, environment and angular functions. Linear interpolation is performed between adjacent table entries. The table length is chosen to be accurate within \( 10^{-6} \) with respect to the \textit{tersoff} style energy. The \textit{tersoff/table} should give better performance in terms of speed.

Only a single pair\_coeff command is used with the \textit{tersoff} style which specifies a Tersoff potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying \( N \) additional arguments after the filename in the pair\_coeff command, where \( N \) is the number of LAMMPS atom types:

- filename
- \( N \) element names = mapping of Tersoff elements to atom types

As an example, imagine the SiC.tersoff file has Tersoff values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair\_coeff command:

```
pair_coeff * * SiC.tersoff Si Si Si C
```

The 1st 2 arguments must be ** so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the Tersoff file. The final C argument maps LAMMPS atom type 4 to the C element in the Tersoff file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a tersoff potential is used as part of the hybrid pair style. The NULL values are
placeholders for atom types that will be used with other potentials.

Tersoff files in the potentials directory of the LAMMPS distribution have a "tersoff" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2 (the atom bonded to the center atom)
- element 3 (the atom influencing the 1-2 bond in a bond-order sense)
- m
- gamma
- lambda3 (1/distance units)
- c
- d
- costheta0 (can be a value < -1 or > 1)
- n
- beta
- lambda2 (1/distance units)
- B (energy units)
- R (distance units)
- D (distance units)
- lambda1 (1/distance units)
- A (energy units)

The n, beta, lambda2, B, lambda1, and A parameters are only used for two-body interactions. The m, gamma, lambda3, c, d, and costheta0 parameters are only used for three-body interactions. The R and D parameters are used for both two-body and three-body interactions. The non-annotated parameters are unitless. The value of m must be 3 or 1.

The Tersoff potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify Tersoff parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction and it is bonded to the 2nd atom and the bond is influenced by the 3rd atom. Thus an entry for SiCC means Si bonded to a C with another C atom influencing the bond. Thus three-body parameters for SiCSi and SiSiC entries will not, in general, be the same. The parameters used for the two-body interaction come from the entry where the 2nd element is repeated. Thus the two-body parameters for Si interacting with C, comes from the SiCC entry.

The parameters used for a particular three-body interaction come from the entry with the corresponding three elements. The parameters used only for two-body interactions (n, beta, lambda2, B, lambda1, and A) in entries whose 2nd and 3rd element are different (e.g. SiCSi) are not used for anything and can be set to 0.0 if desired.

Note that the twobody parameters in entries such as SiCC and CSiSi are often the same, due to the common use of symmetric mixing rules, but this is not always the case. For example, the beta and n parameters in Tersoff_2 (Tersoff_2) are not symmetric.

We chose the above form so as to enable users to define all commonly used variants of the Tersoff potential. In
particular, our form reduces to the original Tersoff form when \( m = 3 \) and \( \gamma = 1 \), while it reduces to the form of Albe et al. when \( \beta = 1 \) and \( m = 1 \). Note that in the current Tersoff implementation in LAMMPS, \( m \) must be specified as either 3 or 1. Tersoff used a slightly different but equivalent form for alloys, which we will refer to as Tersoff_2 potential (Tersoff_2). The `tersoff/table` style implements Tersoff_2 parameterization only.

LAMMPS parameter values for Tersoff_2 can be obtained as follows: \( \gamma_{ijk} = \omega_{ik} \), \( \lambda_3 = 0 \) and the value of \( m \) has no effect. The parameters for species \( i \) and \( j \) can be calculated using the Tersoff_2 mixing rules:

\[
\begin{align*}
\lambda_{1,i,j}^i & = \frac{1}{2} (\lambda_1^i + \lambda_1^j) \\
\lambda_{2,i,j}^i & = \frac{1}{2} (\lambda_2^i + \lambda_2^j) \\
A_{i,j} & = (A_i A_j)^{1/2} \\
B_{i,j} & = \chi_{ij} (B_i B_j)^{1/2} \\
R_{i,j} & = (R_i R_j)^{1/2} \\
S_{i,j} & = (S_i S_j)^{1/2}
\end{align*}
\]

Tersoff_2 parameters \( R \) and \( S \) must be converted to the LAMMPS parameters \( R \) and \( D \) (\( R \) is different in both forms), using the following relations: \( R = (R' + S')/2 \) and \( D = (S' - R')/2 \), where the primes indicate the Tersoff_2 parameters.

In the potentials directory, the file `SiCGe.tersoff` provides the LAMMPS parameters for Tersoff's various versions of Si, as well as his alloy parameters for Si, C, and Ge. This file can be used for pure Si, (three different versions), pure C, pure Ge, binary SiC, and binary SiGe. LAMMPS will generate an error if this file is used with any combination involving C and Ge, since there are no entries for the GeC interactions (Tersoff did not publish parameters for this cross-interaction.) Tersoff files are also provided for the SiC alloy (SiC.tersoff) and the GaN (GaN.tersoff) alloys.

Many thanks to Rutuparna Narulkar, David Farrell, and Xiaowang Zhou for helping clarify how Tersoff parameters for alloys have been defined in various papers.

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Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.
Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I ≠ J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

Restrictions:

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair style requires the newton setting to be "on" for pair interactions.

The Tersoff potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the Tersoff potential with any LAMMPS units, but you would need to create your own Tersoff potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none


(Tersoff_2) J. Tersoff, Phys Rev B, 39, 5566 (1989); errata (PRB 41, 3248)
pair_style tersoff/zbl command

pair_style tersoff/zbl/omp command

Syntax:

pair_style tersoff/zbl

Examples:

pair_style tersoff/zbl
pair_coeff * * SiC.tersoff.zbl Si C Si

Description:

The tersoff/zbl style computes a 3-body Tersoff potential (Tersoff_1) with a close-separation pairwise modification based on a Coulomb potential and the Ziegler-Biersack-Littmark universal screening function (ZBL), giving the energy E of a system of atoms as
\[ E = \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij} \]

\[ V_{ij} = (1 - f_F(r_{ij})) V_{ij}^{ZBL} + f_F(r_{ij}) V_{ij}^{Tersoff} \]

\[ f_F(r_{ij}) = \frac{1}{1 + e^{-A_F(r_{ij} - r_C)}} \]

\[ V_{ij}^{ZBL} = \frac{1}{4\pi\varepsilon_0} \frac{Z_1 Z_2 e^2}{r_{ij}} \phi(r_{ij}/a) \]

\[ a = \frac{0.8854 a_0}{Z_1^{0.23} + Z_2^{0.23}} \]

\[ \phi(x) = 0.1818 e^{-3.2x} + 0.5099 e^{-0.9423x} + 0.2802 e^{-0.4029x} + 0.02817 e^{-0.20} \]

\[ V_{ij}^{Tersoff} = f_C(r_{ij}) [f_R(r_{ij}) + b_{ij} f_A(r_{ij})] \]

\[ f_C(r) = \begin{cases} 
1 & : r < R - D \\
\frac{1}{2} - \frac{1}{2} \sin \left( \frac{\pi r - R}{2D} \right) & : R - D < r < R + D \\
0 & : r > R + D 
\end{cases} \]

\[ f_R(r) = A \exp(-\lambda_1 r) \]

\[ f_A(r) = -B \exp(-\lambda_2 r) \]

\[ b_{ij} = (1 + \beta^n \zeta_{ij}^n)^{-\frac{1}{2n}} \]

\[ \zeta_{ij} = \sum_{k \neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp \left[ \lambda_3^3 (r_{ij} - r_{ik})^m \right] \]

\[ g(\theta) = \gamma_{ijk} \left( 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (\cos \theta - \cos \theta_0)^2} \right) \]
The \( f_F \) term is a fermi-like function used to smoothly connect the ZBL repulsive potential with the Tersoff potential. There are 2 parameters used to adjust it: \( A_F \) and \( r_C \). \( A_F \) controls how "sharp" the transition is between the two, and \( r_C \) is essentially the cutoff for the ZBL potential.

For the ZBL portion, there are two terms. The first is the Coulomb repulsive term, with \( Z_1, Z_2 \) as the number of protons in each nucleus, \( e \) as the electron charge (1 for metal and real units) and \( \epsilon_0 \) as the permittivity of vacuum. The second part is the ZBL universal screening function, with \( a_0 \) being the Bohr radius (typically 0.529 Angstroms), and the remainder of the coefficients provided by the original paper. This screening function should be applicable to most systems. However, it is only accurate for small separations (i.e. less than 1 Angstrom).

For the Tersoff portion, \( f_R \) is a two-body term and \( f_A \) includes three-body interactions. The summations in the formula are over all neighbors \( J \) and \( K \) of atom \( I \) within a cutoff distance = \( R + D \).

Only a single pair_coeff command is used with the *tersoff/zbl* style which specifies a Tersoff/ZBL potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Tersoff/ZBL elements to atom types

As an example, imagine the SiC.tersoff.zbl file has Tersoff/ZBL values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.tersoff Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the Tersoff/ZBL file. The final C argument maps LAMMPS atom type 4 to the C element in the Tersoff/ZBL file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *tersoff/zbl* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Tersoff/ZBL files in the *potentials* directory of the LAMMPS distribution have a ".tersoff.zbl" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2 (the atom bonded to the center atom)
- element 3 (the atom influencing the 1-2 bond in a bond-order sense)
- \( m \)
- \( \gamma \)
- \( \lambda_3 \) (1/distance units)
- \( c \)
- \( d \)
- \( \cos \theta_0 \) (can be a value < -1 or > 1)
- \( n \)
- \( \beta \)
- \( \lambda_2 \) (1/distance units)
- \( B \) (energy units)
- \( R \) (distance units)
- \( D \) (distance units)
- \( \lambda_1 \) (1/distance units)
- \( A \) (energy units)
The $n$, $\beta$, $\lambda_2$, $B$, $\lambda_1$, and $A$ parameters are only used for two-body interactions. The $m$, $\gamma$, $\lambda_3$, $c$, $d$, and $\cos \theta_0$ parameters are only used for three-body interactions. The $R$ and $D$ parameters are used for both two-body and three-body interactions. The $Z_i, Z_j$, $Z_{BLcut}$, $Z_{BLexp}scale$ parameters are used in the ZBL repulsive portion of the potential and in the Fermi-like function. The non-annotated parameters are unitless. The value of $m$ must be 3 or 1.

The Tersoff/ZBL potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify Tersoff parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction and it is bonded to the 2nd atom and the bond is influenced by the 3rd atom. Thus an entry for SiCC means Si bonded to a C with another C atom influencing the bond. Thus three-body parameters for SiCSi and SiSiC entries will not, in general, be the same. The parameters used for the two-body interaction come from the entry where the 2nd element is repeated. Thus the two-body parameters for Si interacting with C comes from the SiCC entry. By symmetry, the two-body parameters in the SiCC and CSiSi entries should thus be the same. The parameters used for a particular three-body interaction come from the entry with the corresponding three elements. The parameters used only for two-body interactions ($n$, $\beta$, $\lambda_2$, $B$, $\lambda_1$, and $A$) in entries whose 2nd and 3rd element are different (e.g. SiCSi) are not used for anything and can be set to 0.0 if desired.

We chose the above form so as to enable users to define all commonly used variants of the Tersoff portion of the potential. In particular, our form reduces to the original Tersoff form when $m = 3$ and $\gamma = 1$, while it reduces to the form of Albe et al. when $\beta = 1$ and $m = 1$. Note that in the current Tersoff implementation in LAMMPS, $m$ must be specified as either 3 or 1. Tersoff used a slightly different but equivalent form for alloys, which we will refer to as Tersoff_2 potential (Tersoff_2).

LAMMPS parameter values for Tersoff_2 can be obtained as follows: $\gamma = 1$, just as for Tersoff_1, but now $\lambda_3 = 0$ and the value of $m$ has no effect. The parameters for species $i$ and $j$ can be calculated using the Tersoff_2 mixing rules:
\[ \lambda_{1,ij} = \frac{1}{2}(\lambda_{1,i} + \lambda_{1,j}) \]
\[ \lambda_{2,ij} = \frac{1}{2}(\lambda_{2,i} + \lambda_{2,j}) \]
\[ A_{i,j} = (A_{i,i}A_{j,j})^{1/2} \]
\[ B_{i,j} = \chi_{ij}(B_{i,i}B_{j,j})^{1/2} \]
\[ R_{i,j} = (R_{i,i}R_{j,j})^{1/2} \]
\[ S_{i,j} = (S_{i,i}S_{j,j})^{1/2} \]

Values not shown are determined by the first atom type. Finally, the Tersoff_2 parameters R and S must be converted to the LAMMPS parameters R and D (R is different in both forms), using the following relations: \( R = \frac{(R'+S')}{2} \) and \( D = \frac{(S'-R')}{2} \), where the primes indicate the Tersoff_2 parameters.

In the potentials directory, the file SiCGe.tersoff provides the LAMMPS parameters for Tersoff's various versions of Si, as well as his alloy parameters for Si, C, and Ge. This file can be used for pure Si, (three different versions), pure C, pure Ge, binary SiC, and binary SiGe. LAMMPS will generate an error if this file is used with any combination involving C and Ge, since there are no entries for the GeC interactions (Tersoff did not publish parameters for this cross-interaction.) Tersoff files are also provided for the SiC alloy (SiC.tersoff) and the GaN (GaN.tersoff) alloys.

Many thanks to Rutuparna Narulkar, David Farrell, and Xiaowang Zhou for helping clarify how Tersoff parameters for alloys have been defined in various papers. Also thanks to Ram Devanathan for providing the base ZBL implementation.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs IJ and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.
This pair style does not support the `pair_modify` shift, table, and tail options.

This pair style does not write its information to `binary restart files`, since it is stored in potential files. Thus, you need to re-specify the `pair_style` and `pair_coeff` commands in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner, middle, outer` keywords.

**Restrictions:**

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair style requires the `newton` setting to be "on" for pair interactions.

The Tersoff/ZBL potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the Tersoff potential with any LAMMPS units, but you would need to create your own Tersoff potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

**Related commands:**

`pair_coeff`

**Default:** none

---


pair_style tri/lj command

pair_style tri/lj/omp command

Syntax:

pair_style tri/lj cutoff

cutoff = global cutoff for interactions (distance units)

Examples:

pair_style tri/lj 3.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.5 2.5

Description:

Style tri/lj treats particles which are triangles as a set of small spherical particles that tile the triangle surface as explained below. Interactions between two triangles, each with N1 and N2 spherical particles, are calculated as the pairwise sum of N1*N2 Lennard-Jones interactions. Interactions between a triangle with N spherical particles and a point particle are treated as the pairwise sum of N Lennard-Jones interactions. See the pair_style lj/cut doc page for the definition of Lennard-Jones interactions.

The cutoff distance for an interaction between 2 triangles, or between a triangle and a point particle, is calculated from the position of the triangle (its centroid), not between pairs of individual spheres comprising the triangle. Thus an interaction is either calculated in its entirety or not at all.

The set of non-overlapping spherical particles that represent a triangle, for purposes of this pair style, are generated in the following manner. Assume the triangle is of type I, and sigma_II has been specified. We want a set of spheres with centers in the plane of the triangle, none of them larger in diameter than sigma_II, which completely cover the triangle's area, but with minimal overlap and a minimal total number of spheres. This is done in a recursive manner. Place a sphere at the centroid of the original triangle. Calculate what diameter it must have to just cover all 3 corner points of the triangle. If that diameter is equal to or smaller than sigma_II, then include a sphere of the calculated diameter in the set of covering spheres. If the diameter is larger than sigma_II, then split the triangle into 2 triangles by bisecting its longest side. Repeat the process on each sub-triangle, recursing as far as needed to generate a set of covering spheres. When finished, the original criteria are met, and the set of covering spheres should be near minimal in number and overlap, at least for input triangles with a reasonable aspect-ratio.

The LJ interaction between 2 spheres on different triangles of types I,J is computed with an arithmetic mixing of the sigma values of the 2 spheres and using the specified epsilon value for I,J atom types. Note that because the sigma values for triangles spheres is computed using only sigma_II values, specific to the triangles's type, this means that any specified sigma_IJ values (for I != J) are effectively ignored.

For style tri/lj, the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- epsilon (energy units)
The last coefficient is optional. If not specified, the global cutoff is used.

Styles with a *cuda*, *gpu*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix* command-line switch when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the *pair_modify* shift, table, and tail options.

This pair style does not write its information to binary restart files.

This pair style can only be used via the *pair* keyword of the *run_style respa* command. It does not support the *inner, middle, outer* keywords.

**Restrictions:**

This style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Defining particles to be triangles so they participate in tri/tri or tri/particle interactions requires the use the *atom_style tri* command.

**Related commands:**

pair_coeff, pair_style line/lj

**Default:** none
**pair_write command**

**Syntax:**

```
pair_write itype jtype N style inner outer file keyword Qi Qj
```

- `itype, jtype` = 2 atom types
- `N` = # of values
- `style` = `r` or `rsq` or `bitmap`
- `inner, outer` = inner and outer cutoff (distance units)
- `file` = name of file to write values to
- `keyword` = section name in file for this set of tabulated values
- `Qi, Qj` = 2 atom charges (charge units) (optional)

**Examples:**

```
pair_write 1 3 500 r 1.0 10.0 table.txt LJ
pair_write 1 1 1000 rsq 2.0 8.0 table.txt Yukawa_1_1 -0.5 0.5
```

**Description:**

Write energy and force values to a file as a function of distance for the currently defined pair potential. This is useful for plotting the potential function or otherwise debugging its values. If the file already exists, the table of values is appended to the end of the file to allow multiple tables of energy and force to be included in one file.

The energy and force values are computed at distances from inner to outer for 2 interacting atoms of type `itype` and `jtype`, using the appropriate `pair_coeff` coefficients. If the style is `r`, then `N` distances are used, evenly spaced in `r`; if the style is `rsq`, `N` distances are used, evenly spaced in `r^2`.

For example, for `N = 7`, style = `r`, inner = 1.0, and outer = 4.0, values are computed at `r = 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0`.

If the style is `bitmap`, then `2^N` values are written to the file in a format and order consistent with how they are read in by the `pair_coeff` command for pair style `table`. For reasonable accuracy in a bitmapped table, choose `N >= 12`, an `inner` value that is smaller than the distance of closest approach of 2 atoms, and an `outer` value <= cutoff of the potential.

If the pair potential is computed between charged atoms, the charges of the pair of interacting atoms can optionally be specified. If not specified, values of `Qi = Qj = 1.0` are used.

The file is written in the format used as input for the `pair_style table` option with `keyword` as the section name. Each line written to the file lists an index number (1-N), a distance (in distance units), an energy (in energy units), and a force (in force units).

**Restrictions:**

All force field coefficients for pair and other kinds of interactions must be set before this command can be invoked.

Due to how the pairwise force is computed, an inner value > 0.0 must be specified even if the potential has a finite
value at \( r = 0.0 \).

For EAM potentials, the pair_write command only tabulates the pairwise portion of the potential, not the embedding portion.

**Related commands:**

`pair_style`, `pair_coeff`

**Default:** none
**pair_style yukawa command**

**pair_style yukawa/gpu command**

**pair_style yukawa/omp command**

**Syntax:**

```
pair_style yukawa kappa cutoff
```

- kappa = screening length (inverse distance units)
- cutoff = global cutoff for Yukawa interactions (distance units)

**Examples:**

```
pair_style yukawa 2.0 2.5
pair_coeff 1 1 100.0 2.3
pair_coeff * * 100.0
```

**Description:**

Style yukawa computes pairwise interactions with the formula

\[
E = A \frac{e^{-\kappa r}}{r} \quad r < r_c
\]

Rc is the cutoff.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- A (energy*distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global yukawa cutoff is used.

---

Styles with a cuda, gpu, omp, or opt suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input...
 See Section accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. The default mix value is geometric. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the pair keyword of the run_style respa command. It does not support the inner, middle, outer keywords.

**Restrictions:** none

**Related commands:**

pair_coeff

**Default:** none
pair_style yukawa/colloid command

pair_style yukawa/colloid/gpu command

pair_style yukawa/colloid/omp command

Syntax:

pair_style yukawa/colloid kappa cutoff

• kappa = screening length (inverse distance units)
• cutoff = global cutoff for colloidal Yukawa interactions (distance units)

Examples:

pair_style yukawa/colloid 2.0 2.5
pair_coeff 1 1 100.0 2.3
pair_coeff * * 100.0

Description:

Style yukawa/colloid computes pairwise interactions with the formula

\[ E = \frac{A}{\kappa} e^{-\kappa(r-(r_i+r_j))} \quad r < r_c \]

where \( r_i \) and \( r_j \) are the radii of the two particles and \( r_c \) is the cutoff.

In contrast to pair_style yukawa, this functional form arises from the Coulombic interaction between two colloid particles, screened due to the presence of an electrolyte. Pair_style yukawa is a screened Coulombic potential between two point-charges and uses no such approximation.

This potential applies to nearby particle pairs for which the Derjagin approximation holds, meaning \( h \ll r_i + r_j \), where \( h \) is the surface-to-surface separation of the two particles.

When used in combination with pair_style colloid, the two terms become the so-called DLVO potential, which combines electrostatic repulsion and van der Waals attraction.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

• A (energy/distance units)
• cutoff (distance units)

The prefactor A is determined from the relationship between surface charge and surface potential due to the presence of electrolyte. Note that the A for this potential style has different units than the A used in pair_style.
The Yukawa potential, for low surface potentials, can be written as:

$$A = 2 \times \pi \times R \times \varepsilon \times \varepsilon_0 \times \kappa \times \psi^2$$

where

- $R$ = colloid radius (distance units)
- $\varepsilon_0$ = permittivity of free space (charge$^2$/energy/distance units)
- $\varepsilon$ = relative permittivity of fluid medium (dimensionless)
- $\kappa$ = inverse screening length (1/distance units)
- $\psi$ = surface potential (energy/charge units)

The last coefficient is optional. If not specified, the global Yukawa/colloid cutoff is used.

Styles with a `cuda`, `gpu`, `omp`, or `opt` suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the `-suffix` command-line switch when you invoke LAMMPS, or you can use the `suffix` command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

**Mixing, shift, table, tail correction, restart, rRESPA info:**

For atom type pairs I,J and I $\neq$ J, the $A$ coefficient and cutoff distance for this pair style can be mixed. $A$ is an energy value mixed like a LJ epsilon. The default mix value is geometric. See the "pair_modify" command for details.

This pair style supports the `pair_modify` shift option for the energy of the pair interaction.

The `pair_modify` table option is not relevant for this pair style.

This pair style does not support the `pair_modify` tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so `pair_style` and `pair_coeff` commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the `pair` keyword of the `run_style respa` command. It does not support the `inner, middle, outer` keywords.

**Restrictions:**

This style is part of the COLLOID package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.
This pair style requires that atoms be finite-size spheres with a diameter, as defined by the `atom_style sphere` command.

Per-particle polydispersity is not yet supported by this pair style; per-type polydispersity is allowed. This means all particles of the same type must have the same diameter. Each type can have a different diameter.

**Related commands:**

pair_coeff

**Default:** none
partition command

Syntax:

partition style N command ...

- style = yes or no
- N = partition number (see asterisk form below)
- command = any LAMMPS command

Examples:

partition yes 1 processors 4 10 6
partition no 5 print "Active partition"
partition yes *5 fix all nve
partition yes 6* fix all nvt temp 1.0 1.0 0.1

Description:

This command invokes the specified command on a subset of the partitions of processors you have defined via the -partition command-line switch. See Section_start 6 for an explanation of the switch.

Normally, every input script command in your script is invoked by every partition. This behavior can be modified by defining world- or universe-style variables that have different values for each partition. This mechanism can be used to cause your script to jump to different input script files on different partitions, if such a variable is used in a jump command.

The "partition" command is another mechanism for having as input script operate differently on different partitions. It is basically a prefix on any LAMMPS command. The command will only be invoked on the partition(s) specified by the style and N arguments.

If the style is yes, the command will be invoked on any partition which matches the N argument. If the style is no the command will be invoked on all the partitions which do not match the Np argument.

Partitions are numbered from 1 to Np, where Np is the number of partitions specified by the -partition command-line switch.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to span a range of partition numbers. This takes the form "*" or "*n" or "n*" or "m*n". An asterisk with no numeric values means all partitions from 1 to Np. A leading asterisk means all partitions from 1 to n (inclusive). A trailing asterisk means all partitions from n to Np (inclusive). A middle asterisk means all partitions from m to n (inclusive).

This command can be useful for the "run_style verlet/split" command which imposed requirements on how the processors command lays out a 3d grid of processors in each of 2 partitions.

Restrictions: none

Related commands:

run_style verlet/split
Default: none
**prd command**

**Syntax:**

```
prd N t_event n_dephase t_dephase t_correlate compute-ID seed keyword value ...
```

- **N** = # of timesteps to run (not including dephasing/quenching)
- **t_event** = timestep interval between event checks
- **n_dephase** = number of velocity randomizations to perform in each dephase run
- **t_dephase** = number of timesteps to run dynamics after each velocity randomization during dephase
- **t_correlate** = number of timesteps within which 2 consecutive events are considered to be correlated
- **compute-ID** = ID of the compute used for event detection
- **random_seed** = random # seed (positive integer)
- zero or more keyword/value pairs may be appended
- **keyword** = *min* or *temp* or *vel*

  - **min values** = etol ftol maxiter maxeval
    - **etol** = stopping tolerance for energy, used in quenching
    - **ftol** = stopping tolerance for force, used in quenching
    - **maxiter** = max iterations of minimize, used in quenching
    - **maxeval** = max number of force/energy evaluations, used in quenching
  - **temp value** = Tdephase
    - **Tdephase** = target temperature for velocity randomization, used in dephasing
  - **vel values** = loop dist
    - **loop** = all or local or geom, used in dephasing
    - **dist** = uniform or gaussian, used in dephasing

**Examples:**

```
prd 5000 100 10 10 100 1 54982
prd 5000 100 10 10 100 1 54982 min 0.1 0.1 100 200
```

**Description:**

Run a parallel replica dynamics (PRD) simulation using multiple replicas of a system. One or more replicas can be used.

PRD is described in [this paper](#) by Art Voter. It is a method for performing accelerated dynamics that is suitable for infrequent-event systems that obey first-order kinetics. A good overview of accelerated dynamics methods for such systems is given in [this review paper](#) from the same group. To quote from the paper: "The dynamical evolution is characterized by vibrational excursions within a potential basin, punctuated by occasional transitions between basins." The transition probability is characterized by \( p(t) = k \cdot \exp(-kt) \) where \( k \) is the rate constant. Running multiple replicas gives an effective enhancement in the timescale spanned by the multiple simulations, while waiting for an event to occur.

Each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the -partition command-line switch; see Section_start 6 of the manual. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g you can run a 10-replica simulation on one or two processors. For PRD, this makes little sense, since this offers no effective parallel speed-up in searching for infrequent events. See Section_howto 5 of the manual for further discussion.
When a PRD simulation is performed, it is assumed that each replica is running the same model, though LAMMPS does not check for this. I.e. the simulation domain, the number of atoms, the interaction potentials, etc should be the same for every replica.

A PRD run has several stages, which are repeated each time an "event" occurs in one of the replicas, as defined below. The logic for a PRD run is as follows:

```
while (time remains):
    dephase for n_dephase*t_dephase steps
    until (event occurs on some replica):
        run dynamics for t_event steps
        quench
        check for uncorrelated event on any replica
    until (no correlated event occurs):
        run dynamics for t_correlate steps
        quench
        check for correlated event on this replica
    event replica shares state with all replicas
```

Before this loop begins, the state of the system on replica 0 is shared with all replicas, so that all replicas begin from the same initial state. The first potential energy basin is identified by quenching (an energy minimization, see below) the initial state and storing the resulting coordinates for reference.

In the first stage, dephasing is performed by each replica independently to eliminate correlations between replicas. This is done by choosing a random set of velocities, based on the random_seed that is specified, and running t_dephase timesteps of dynamics. This is repeated n_dephase times. If the temp keyword is not specified, the target temperature for velocity randomization for each replica is the current temperature of that replica. Otherwise, it is the specified Tdephase temperature. The style of velocity randomization is controlled using the keyword vel with arguments that have the same meaning as their counterparts in the velocity command.

In the second stage, each replica runs dynamics continuously, stopping every t_event steps to check if a transition event has occurred. This check is performed by quenching the system and comparing the resulting atom coordinates to the coordinates from the previous basin. The first time through the PRD loop, the "previous basin" is the set of quenched coordinates from the initial state of the system.

A quench is an energy minimization and is performed by whichever algorithm has been defined by the min_style command. Minimization parameters may be set via the min_modify command and by the min keyword of the PRD command. The latter are the settings that would be used with the minimize command. Note that typically, you do not need to perform a highly-converged minimization to detect a transition event.

The event check is performed by a compute with the specified compute-ID. Currently there is only one compute that works with the PRD command, which is the compute event/displace command. Other event-checking computes may be added. Compute event/displace checks whether any atom in the compute group has moved further than a specified threshold distance. If so, an "event" has occurred.

In the third stage, the replica on which the event occurred (event replica) continues to run dynamics to search for correlated events. This is done by running dynamics for t_correlate steps, quenching every t_event steps, and checking if another event has occurred. The first time no correlated event occurs, the final state of the event replica is shared with all replicas, the new basin reference coordinates are updated with the quenched state, and the outer loop begins again. While the replica event is searching for correlated events, all the other replicas also run dynamics and event checking with the same schedule, but the final states are always overwritten by the state of the event replica.
Four kinds of output can be generated during a PRD run: event statistics, thermodynamic output by each replica, dump files, and restart files.

When running with multiple partitions (each of which is a replica in this case), the print-out to the screen and master log.lammps file is limited to event statistics. Note that if a PRD run is performed on only a single replica then the event statistics will be intermixed with the usual thermodynamic output discussed below.

The quantities printed each time an event occurs are the timestep, CPU time, clock, event number, a correlation flag, the number of coincident events, and the replica number of the chosen event.

The timestep is the usual LAMMPS timestep, except that time does not advance during dephasing or quenches, but only during dynamics. Note that are two kinds of dynamics in the PRD loop listed above. The first is when all replicas are performing independent dynamics. The second is when correlated events are being searched for and only one replica is running dynamics.

The CPU time is the total processor time since the start of the PRD run.

The clock is the same as the timestep except that it advances by M steps every timestep during the first kind of dynamics when the M replicas are running independently. The clock represents the real time that effectively elapses during a PRD simulation of N steps on M replicas. If most of the PRD run is spent in the second stage of the loop above, searching for infrequent events, then the clock will advance nearly N*M steps. Note the clock time between events will be drawn from p(t).

The event number is a counter that increments with each event, whether it is uncorrelated or correlated.

The correlation flag will be 0 when an uncorrelated event occurs during the second stage of the loop listed above, i.e. when all replicas are running independently. The correlation flag will be 1 when a correlated event occurs during the third stage of the loop listed above, i.e. when only one replica is running dynamics.

When more than one replica detects an event at the end of the second stage, then one of them is chosen at random. The number of coincident events is the number of replicas that detected an event. Normally, we expect this value to be 1. If it is often greater than 1, then either the number of replicas is too large, or \( t_{\text{event}} \) is too large.

The replica number is the ID of the replica (from 0 to M-1) that found the event.

When running on multiple partitions, LAMMPS produces additional log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For the PRD command, these contain the thermodynamic output for each replica. You will see short runs and minimizations corresponding to the dynamics and quench operations of the loop listed above. The timestep will be reset appropriately depending on whether the operation advances time or not.

After the PRD command completes, timing statistics for the PRD run are printed in each replica’s log file, giving a breakdown of how much CPU time was spent in each stage (dephasing, dynamics, quenching, etc).

Any dump files defined in the input script, will be written to during a PRD run at timesteps corresponding to both uncorrelated and correlated events. This means the the requested dump frequency in the dump command is ignored. There will be one dump file (per dump command) created for all partitions.

The atom coordinates of the dump snapshot are those of the minimum energy configuration resulting from quenching following a transition event. The timesteps written into the dump files correspond to the timestep at which the event occurred and NOT the clock. A dump snapshot corresponding to the initial minimum state used for event detection is written to the dump file at the beginning of each PRD run.
If the \texttt{restart} command is used, a single restart file for all the partitions is generated, which allows a PRD run to be continued by a new input script in the usual manner.

The restart file is generated at the end of the loop listed above. If no correlated events are found, this means it contains a snapshot of the system at time $T + t_{correlate}$, where $T$ is the time at which the uncorrelated event occurred. If correlated events were found, then it contains a snapshot of the system at time $T + t_{correlate}$, where $T$ is the time of the last correlated event.

The restart frequency specified in the \texttt{restart} command is interpreted differently when performing a PRD run. It does not mean the timestep interval between restart files. Instead it means an event interval for uncorrelated events. Thus a frequency of 1 means write a restart file every time an uncorrelated event occurs. A frequency of 10 means write a restart file every 10th uncorrelated event.

When an input script reads a restart file from a previous PRD run, the new script can be run on a different number of replicas or processors. However, it is assumed that $t_{correlate}$ in the new PRD command is the same as it was previously. If not, the calculation of the "clock" value for the first event in the new run will be slightly off.

\textbf{Restrictions:}

This command can only be used if LAMMPS was built with the REPLICA package. See the \texttt{Making LAMMPS} section for more info on packages.

\textit{N} and \textit{t_correlate} settings must be integer multiples of \textit{t_event}.

Runs restarted from restart file written during a PRD run will not produce identical results due to changes in the random numbers used for dephasing.

This command cannot be used when any fixes are defined that keep track of elapsed time to perform time-dependent operations. Examples include the "ave" fixes such as \texttt{fix ave/spatial}. Also \texttt{fix dt/reset} and \texttt{fix deposit}.

\textbf{Related commands:}

\texttt{compute event/displace, min_modify, min_style, run_style, minimize, velocity, temper, neb, tad}

\textbf{Default:}

The option defaults are \textit{min} = 0.1 0.1 40 50, no \textit{temp} setting, and \textit{vel} = \textit{geom gaussian}.


print command

Syntax:

print str

- str = text string to print, which may contain variables

Examples:

print "Done with equilibration"
print Vol=$v
print "The system volume is now $v"
print 'The system volume is now $v'

Description:

Print a text string to the screen and logfile. One line of output is generated. If the string has white space in it (spaces, tabs, etc), then you must enclose it in quotes so that it is treated as a single argument. If variables are included in the string, they will be evaluated and their current values printed.

If you want the print command to be executed multiple times (with changing variable values), there are 3 options. First, consider using the fix print command, which will print a string periodically during a simulation. Second, the print command can be used as an argument to the every option of the run command. Third, the print command could appear in a section of the input script that is looped over (see the jump and next commands).

See the variable command for a description of equal style variables which are typically the most useful ones to use with the print command. Equal-style variables can calculate formulas involving mathematical operations, atom properties, group properties, thermodynamic properties, global values calculated by a compute or fix, or references to other variables.

Restrictions: none

Related commands:

fix print, variable

Default: none
processors command

Syntax:

processors Px Py Pz keyword args ...

- Px,Py,Pz = # of processors in each dimension of 3d grid overlaying the simulation domain
- zero or more keyword/arg pairs may be appended
- keyword = grid or map or part or file

grid arg = gstyle params ...
- gstyle = onelevel or twolevel or numa or custom
  - onelevel params = none
  - twolevel params = Nc Cx Cy Cz
    - Nc = number of cores per node
    - Cx,Cy,Cz = # of cores in each dimension of 3d sub-grid assigned to each node
  - numa params = none
  - custom params = infile
    - infile = file containing grid layout

map arg = cart or cart/reorder or xyz or xzy or yxz or yzx or zxy or zyx
- cart = use MPI_Cart() methods to map processors to 3d grid with reorder = 0
- cart/reorder = use MPI_Cart() methods to map processors to 3d grid with reorder = 1
- xyz,xzy,yxz,yzx,zxy,zyx = map processors to 3d grid in IJK ordering

numa arg = none

part args = Psend Precv cstyle
- Psend = partition # (1 to Np) which will send its processor layout
- Precv = partition # (1 to Np) which will recv the processor layout
- cstyle = multiple
  - multiple = Psend grid will be multiple of Precv grid in each dimension

file arg = outfile
- outfile = name of file to write 3d grid of processors to

Examples:

processors * * 5
processors 2 4 4
processors * * 8 map xyz
processors * * * grid numa
processors * * * grid twolevel 4 * * 1
processors 4 8 16 grid custom myfile
processors * * * part 1 2 multiple

Description:

Specify how processors are mapped as a 3d logical grid to the global simulation box. This involves 2 steps. First if there are P processors it means choosing a factorization P = Px by Py by Pz so that there are Px processors in the x dimension, and similarly for the y and z dimensions. Second, the P processors are mapped to the logical 3d grid. The arguments to this command control each of these 2 steps.

The Px, Py, Pz parameters affect the factorization. Any of the 3 parameters can be specified with an asterisk "*", which means LAMMPS will choose the number of processors in that dimension of the grid. It will do this based on the size and shape of the global simulation box so as to minimize the surface-to-volume ratio of each processor's sub-domain.
Since LAMMPS does not load-balance by changing the grid of 3d processors on-the-fly, choosing explicit values for Px or Py or Pz can be used to override the LAMMPS default if it is known to be sub-optimal for a particular problem. E.g. a problem where the extent of atoms will change dramatically in a particular dimension over the course of the simulation.

The product of Px, Py, Pz must equal P, the total # of processors LAMMPS is running on. For a 2d simulation, Pz must equal 1.

Note that if you run on a prime number of processors P, then a grid such as 1 x P x 1 will be required, which may incur extra communication costs due to the high surface area of each processor's sub-domain.

Also note that if multiple partitions are being used then P is the number of processors in this partition; see this section for an explanation of the -partition command-line switch. Also note that you can prefix the processors command with the partition command to easily specify different Px,Py,Pz values for different partitions.

You can use the partition command to specify different processor grids for different partitions, e.g.

```
partition yes 1 processors 4 4 4
partition yes 2 processors 2 3 2
```

The grid keyword affects the factorization of P into Px,Py,Pz and it can also affect how the P processor IDs are mapped to the 3d grid of processors.

The onelevel style creates a 3d grid that is compatible with the Px,Py,Pz settings, and which minimizes the surface-to-volume ratio of each processor's sub-domain, as described above. The mapping of processors to the grid is determined by the map keyword setting.

The twolevel style can be used on machines with multicore nodes to minimize off-node communication. It insures that contiguous sub-sections of the 3d grid are assigned to all the cores of a node. For example if Nc is 4, then 2x2x1 or 2x1x2 or 1x2x2 sub-sections of the 3d grid will correspond to the cores of each node. This affects both the factorization and mapping steps.

The Cx, Cy, Cz settings are similar to the Px, Py, Pz settings, only their product should equal Nc. Any of the 3 parameters can be specified with an asterisk "*", which means LAMMPS will choose the number of cores in that dimension of the node's sub-grid. As with Px,Py,Pz, it will do this based on the size and shape of the global simulation box so as to minimize the surface-to-volume ratio of each processor's sub-domain.

IMPORTANT NOTE: For the twolevel style to work correctly, it assumes the MPI ranks of processors LAMMPS is running on are ordered by core and then by node. E.g. if you are running on 2 quad-core nodes, for a total of 8 processors, then it assumes processors 0,1,2,3 are on node 1, and processors 4,5,6,7 are on node 2. This is the default rank ordering for most MPI implementations, but some MPis provide options for this ordering, e.g. via environment variable settings.

The numa style operates similar to the twolevel keyword except that it auto-detects which cores are running on which nodes. Currently, it does this in only 2 levels, but it may be extended in the future to account for socket topology and other non-uniform memory access (NUMA) costs. It also uses a different algorithm than the twolevel keyword for doing the two-level factorization of the simulation box into a 3d processor grid to minimize off-node communication, and it does its own MPI-based mapping of nodes and cores to the logical 3d grid. Thus it may produce a different layout of the processors than the twolevel options.

The numa style will give an error if the number of MPI processes is not divisible by the number of cores used per node, or any of the Px or Py of Pz values is greater than 1.
IMPORTANT NOTE: Unlike the twolevel style, the numa style does not require any particular ordering of MPI ranks in order to work correctly. This is because it auto-detects which processes are running on which nodes.

The custom style uses the file infile to define both the 3d factorization and the mapping of processors to the grid.

The file should have the following format. Any number of initial blank or comment lines (starting with a "#" character) can be present. The first non-blank, non-comment line should have 3 values:

\[ Px \, Py \, Pz \]

These must be compatible with the total number of processors and the Px, Py, Pz settings of the processors command.

This line should be immediately followed by P = Px*Py*Pz lines of the form:

\[ ID \, I \, J \, K \]

where ID is a processor ID (from 0 to P-1) and I,J,K are the processors location in the 3d grid. I must be a number from 1 to Px (inclusive) and similarly for J and K. The P lines can be listed in any order, but no processor ID should appear more than once.

The map keyword affects how the P processor IDs (from 0 to P-1) are mapped to the 3d grid of processors. It is only used by the onelevel and twolevel grid settings.

The cart style uses the family of MPI Cartesian functions to perform the mapping, namely MPI_Cart_create(), MPI_Cart_get(), MPI_Cart_shift(), and MPI_Cart_rank(). It invokes the MPI_Cart_create() function with its reorder flag = 0, so that MPI is not free to reorder the processors.

The cart/reorder style does the same thing as the cart style except it sets the reorder flag to 1, so that MPI can reorder processors if it desires.

The xyz, xzy, yxz, yzx, zxy, and zyx styles are all similar. If the style is IJK, then it maps the P processors to the grid so that the processor ID in the I direction varies fastest, the processor ID in the J direction varies next fastest, and the processor ID in the K direction varies slowest. For example, if you select style xyz and you have a 2x2x2 grid of 8 processors, the assignments of the 8 octants of the simulation domain will be:

\[
\begin{align*}
proc 0 &= \text{lo x, lo y, lo z octant} \\
proc 1 &= \text{hi x, lo y, lo z octant} \\
proc 2 &= \text{lo x, hi y, lo z octant} \\
proc 3 &= \text{hi x, hi y, lo z octant} \\
proc 4 &= \text{lo x, lo y, hi z octant} \\
proc 5 &= \text{hi x, lo y, hi z octant} \\
proc 6 &= \text{lo x, hi y, hi z octant} \\
proc 7 &= \text{hi x, hi y, hi z octant}
\end{align*}
\]

Note that, in principle, an MPI implementation on a particular machine should be aware of both the machine's network topology and the specific subset of processors and nodes that were assigned to your simulation. Thus its MPI_Cart calls can optimize the assignment of MPI processes to the 3d grid to minimize communication costs. In practice, however, few if any MPI implementations actually do this. So it is likely that the cart and cart/reorder styles simply give the same result as one of the IJK styles.

Also note, that for the twolevel grid style, the map setting is used to first map the nodes to the 3d grid, then again to the cores within each node. For the latter step, the cart and cart/reorder styles are not supported, so an xyz style is used in their place.
The part keyword affects the factorization of P into Px, Py, Pz.

It can be useful when running in multi-partition mode, e.g., with the run_style verlet/split command. It specifies a dependency between a sending partition Psend and a receiving partition Precv which is enforced when each is setting up their own mapping of their processors to the simulation box. Each of Psend and Precv must be integers from 1 to Np, where Np is the number of partitions you have defined via the -partition command-line switch.

A "dependency" means that the sending partition will create its 3d logical grid as Px by Py by Pz and after it has done this, it will send the Px, Py, Pz values to the receiving partition. The receiving partition will wait to receive these values before creating its own 3d logical grid and will use the sender's Px, Py, Pz values as a constraint. The nature of the constraint is determined by the cstyle argument.

For a cstyle of multiple, each dimension of the sender's processor grid is required to be an integer multiple of the corresponding dimension in the receiver's processor grid. This is a requirement of the run_style verlet/split command.

For example, assume the sending partition creates a 4x6x10 grid = 240 processor grid. If the receiving partition is running on 80 processors, it could create a 4x2x10 grid, but it will not create a 2x4x10 grid, since in the y-dimension, 6 is not an integer multiple of 4.

IMPORTANT NOTE: If you use the partition command to invoke different "processors" commands on different partitions, and you also use the part keyword, then you must ensure that both the sending and receiving partitions invoke the "processors" command that connects the 2 partitions via the part keyword. LAMMPS cannot easily check for this, but your simulation will likely hang in its setup phase if this error has been made.

The file keyword writes the mapping of the factorization of P processors and their mapping to the 3d grid to the specified file outfile. This is useful to check that you assigned physical processors in the manner you desired, which can be tricky to figure out, especially when running on multiple partitions or on a multicore machine or when the processor ranks were reordered by use of the -reorder command-line switch or due to use of MPI-specific launch options such as a config file.

If you have multiple partitions you should ensure that each one writes to a different file, e.g., using a world-style variable for the filename. The file has a self-explanatory header, followed by one-line per processor in this format:

world-ID universe-ID original-ID: I J K: name

The IDs are the processor's rank in this simulation (the world), the universe (of multiple simulations), and the original MPI communicator used to instantiate LAMMPS, respectively. The world and universe IDs will only be different if you are running on more than one partition; see the -partition command-line switch. The universe and original IDs will only be different if you used the -reorder command-line switch to reorder the processors differently than their rank in the original communicator LAMMPS was instantiated with.

I, J, K are the indices of the processor in the 3d logical grid, each from 1 to Nd, where Nd is the number of processors in that dimension of the grid.

The name is what is returned by a call to MPI_Get_processor_name() and should represent an identifier relevant to the physical processors in your machine. Note that depending on the MPI implementation, multiple cores can have the same name.

Restrictions:
This command cannot be used after the simulation box is defined by a read_data or create_box command. It can be used before a restart file is read to change the 3d processor grid from what is specified in the restart file.

The grid numa keyword only currently works with the map cart option.

The part keyword (for the receiving partition) only works with the grid onelevel or grid twolevel options.

Related commands:

partition, -reorder command-line switch

Default:

The option defaults are Px Py Pz = * * *, grid = onelevel, and map = cart.
quit command

Syntax:

quit

Examples:

quit
if "$n > 10000" then quit

Description:

This command causes LAMMPS to exit, after shutting down all output cleanly.

It can be used as a debug statement in an input script, to terminate the script at some intermediate point.

It can also be used as an invoked command inside the "then" or "else" portion of an if command.

Restrictions: none

Related commands:

if

Default: none
read_data command

Syntax:

read_data file keyword args ...

- file = name of data file to read in
- zero or more keyword/arg pairs may be appended
- keyword = fix

fix args = fix-ID header-string section-string
  fix-ID = ID of fix to process header lines and sections of data file
  header-string = header lines containing this string will be passed to fix
  section-string = section names with this string will be passed to fix

Examples:

read_data data.lj
read_data ../run7/data.polymer.gz
read_data data.protein fix mycmap crossterm CMAP

Description:

Read in a data file containing information LAMMPS needs to run a simulation. The file can be ASCII text or a
gzipped text file (detected by a .gz suffix). This is one of 3 ways to specify initial atom coordinates; see the
read_restart and create_atoms commands for alternative methods.

The structure of the data file is important, though many settings and sections are optional or can come in any
order. See the examples directory for sample data files for different problems.

A data file has a header and a body. The header appears first. The first line of the header is always skipped; it
typically contains a description of the file. Then lines are read one at a time. Lines can have a trailing comment
starting with '#' that is ignored. If the line is blank (only whitespace after comment is deleted), it is skipped. If the
line contains a header keyword, the corresponding value(s) is read from the line. If it doesn't contain a header
keyword, the line begins the body of the file.

The body of the file contains zero or more sections. The first line of a section has only a keyword. The next line is
skipped. The remaining lines of the section contain values. The number of lines depends on the section keyword
as described below. Zero or more blank lines can be used between sections. Sections can appear in any order, with
a few exceptions as noted below.

If the keyword fix is used, it specifies a fix that will be used to process portions of the data file. Any header line
containing header-string and any section with a name containing section-string will be passed to the fix. See the
fix cmap command for an example of a fix that operates in this manner. The doc page for the fix defines the
syntax of the header line(s) and section(s) that it reads from the data file.

The formatting of individual lines in the data file (indentation, spacing between words and numbers) is not
important except that header and section keywords (e.g. atoms, xlo xhi, Masses, Bond Coeffs) must be capitalized
as shown and can't have extra white space between their words - e.g. two spaces or a tab between "Bond" and
"Coeffs" is not valid.
These are the recognized header keywords. Header lines can come in any order. The value(s) are read from the beginning of the line. Thus the keyword *atoms* should be in a line like "1000 atoms"; the keyword *ylo yhi* should be in a line like "-10.0 10.0 ylo yhi"; the keyword *xy xz yz* should be in a line like "0.0 5.0 6.0 xy xz yz". All these settings have a default value of 0, except the lo/hi box size defaults are -0.5 and 0.5. A line need only appear if the value is different than the default.

- **atoms** = # of atoms in system
- **bonds** = # of bonds in system
- **angles** = # of angles in system
- **dihedrals** = # of dihedrals in system
- **impropers** = # of impropers in system
- **atom types** = # of atom types in system
- **bond types** = # of bond types in system
- **angle types** = # of angle types in system
- **dihedral types** = # of dihedral types in system
- **improper types** = # of improper types in system
- **extra bond per atom** = leave space for this many new bonds per atom
- **ellipsoids** = # of ellipsoids in system
- **lines** = # of line segments in system
- **triangles** = # of triangles in system
- **xlo xhi** = simulation box boundaries in x dimension
- **ylo yhi** = simulation box boundaries in y dimension
- **zlo zhi** = simulation box boundaries in z dimension
- **xy xz yz** = simulation box tilt factors for triclinic system

The initial simulation box size is determined by the lo/hi settings. In any dimension, the system may be periodic or non-periodic; see the **boundary** command.

If the *xy xz yz* line does not appear, LAMMPS will set up an axis-aligned (orthogonal) simulation box. If the line does appear, LAMMPS creates a non-orthogonal simulation domain shaped as a parallelepiped with triclinic symmetry. The parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by $A = (xhi-xlo,0,0)$; $B = (xy,yhi-ylo,0)$; $C = (xz,yz,zhi-zlo)$. $Xy,xz,yz$ can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped.

The tilt factors (xy,xz,yz) can not skew the box more than half the distance of the corresponding parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all geometrically equivalent.

See [Section howto 12](#) of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

When a triclinic system is used, the simulation domain must be periodic in any dimensions with a non-zero tilt factor, as defined by the **boundary** command. I.e. if the xy tilt factor is non-zero, then both the x and y dimensions must be periodic. Similarly, x and z must be periodic if xz is non-zero and y and z must be periodic if yz is non-zero. Also note that if your simulation will tilt the box, e.g. via the **fix deform** command, the simulation box must be defined as triclinic, even if the tilt factors are initially 0.0.

For 2d simulations, the *zlo zhi* values should be set to bound the z coords for atoms that appear in the file; the default of -0.5 0.5 is valid if all z coords are 0.0. For 2d triclinic simulations, the xz and yz tilt factors must be 0.0.
If the system is periodic (in a dimension), then atom coordinates can be outside the bounds (in that dimension); they will be remapped (in a periodic sense) back inside the box.

IMPORTANT NOTE: If the system is non-periodic (in a dimension), then all atoms in the data file must have coordinates (in that dimension) that are "greater than or equal to" the lo value and "less than or equal to" the hi value. If the non-periodic dimension is of style "fixed" (see the boundary command), then the atom coords must be strictly "less than" the hi value, due to the way LAMMPS assign atoms to processors. Note that you should not make the lo/hi values radically smaller/larger than the extent of the atoms. For example, if your atoms extend from 0 to 50, you should not specify the box bounds as -10000 and 10000. This is because LAMMPS uses the specified box size to layout the 3d grid of processors. A huge (mostly empty) box will be sub-optimal for performance when using "fixed" boundary conditions (see the boundary command). When using "shrink-wrap" boundary conditions (see the boundary command), a huge (mostly empty) box may cause a parallel simulation to lose atoms the first time that LAMMPS shrink-wraps the box around the atoms.

The "extra bond per atom" setting should be used if new bonds will be added to the system when a simulation runs, e.g. by using the fix bond/create command. This will pre-allocate space in LAMMPS data structures for storing the new bonds.

The "ellipsoids" and "lines" and "triangles" settings are only used with atom_style ellipsoid or line or tri and specifies how many of the atoms are finite-size ellipsoids or lines or triangles; the remainder are point particles. See the discussion of ellipsoidflag and the Ellipsoids section below. See the discussion of lineflag and the Lines section below. See the discussion of triangleflag and the Triangles section below.

These are the section keywords for the body of the file:

- Atoms, Velocities, Masses, Ellipsoids, Lines, Triangles = atom-property sections
- Bonds, Angles, Dihedrals, Impropers = molecular topology sections
- Pair Coeffs, Bond Coeffs, Angle Coeffs, Dihedral Coeffs, Improper Coeffs = force field sections
- BondBond Coeffs, BondAngle Coeffs, MiddleBondTorsion Coeffs, EndBondTorsion Coeffs, AngleTorsion Coeffs, AngleAngleTorsion Coeffs, BondBond13 Coeffs, AngleAngle Coeffs = class 2 force field sections

Each section is listed below in alphabetic order. The format of each section is described including the number of lines it must contain and rules (if any) for where it can appear in the data file.

Any individual line in the various sections can have a trailing comment starting with "#" for annotation purposes. E.g. in the Atoms section:

10 1 17 -1.0 10.0 5.0 6.0   # salt ion

**Angle Coeffs section:**

- one line per angle type
- line syntax: ID coeffs

  ID = angle type (1-N)
  coeffs = list of coeffs

- example:

  6 70 108.5 0 0

The number and meaning of the coefficients are specific to the defined angle style. See the angle_style and angle_coeff commands for details. Coefficients can also be set via the angle_coeff command in the input script.
**AngleAngle Coeffs section:**

- one line per improper type
- line syntax: ID coeffs

  ID = improper type (1-N)  
  coeffs = list of coeffs (see improper_coeff)

**AngleAngleTorsion Coeffs section:**

- one line per dihedral type
- line syntax: ID coeffs

  ID = dihedral type (1-N)  
  coeffs = list of coeffs (see dihedral_coeff)

**Angles section:**

- one line per angle
- line syntax: ID type atom1 atom2 atom3

  ID = number of angle (1-Nangles)  
  type = angle type (1-Nangletype)  
  atom1,atom2,atom3 = IDs of 1st,2nd,3rd atoms in angle

  example:

  2 2 17 29 430

The 3 atoms are ordered linearly within the angle. Thus the central atom (around which the angle is computed) is the atom2 in the list. E.g. H,O,H for a water molecule. The Angles section must appear after the Atoms section. All values in this section must be integers (1, not 1.0).

**AngleTorsion Coeffs section:**

- one line per dihedral type
- line syntax: ID coeffs

  ID = dihedral type (1-N)  
  coeffs = list of coeffs (see dihedral_coeff)

**Atoms section:**

- one line per atom
- line syntax: depends on atom style

An Atoms section must appear in the data file if natoms > 0 in the header section. The atoms can be listed in any order. These are the line formats for each atom style in LAMMPS. As discussed below, each line can optionally have 3 flags (nx,ny,nz) appended to it, which indicate which image of a periodic simulation box the atom is in. These may be important to include for some kinds of analysis.

<table>
<thead>
<tr>
<th>Style</th>
<th>Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>angle</td>
<td>atom-ID molecule-ID atom-type x y z</td>
</tr>
<tr>
<td>atomic</td>
<td>atom-ID atom-type x y z</td>
</tr>
</tbody>
</table>
The keywords have these meanings:

- **atom-ID** = integer ID of atom
- **molecule-ID** = integer ID of molecule the atom belongs to
- **atom-type** = type of atom (1-Ntype)
- **q** = charge on atom (charge units)
- **diameter** = diameter of spherical atom (distance units)
- **ellipsoidflag** = 1 for ellipsoidal particles, 0 for point particles
- **lineflag** = 1 for line segment particles, 0 for point particles
- **triangleflag** = 1 for triangular particles, 0 for point particles
- **density** = density of particle (mass/distance^3 or mass/distance^2 or mass/distance units, depending on dimensionality of particle)
- **volume** = volume of atom (distance^3 units)
- **x,y,z** = coordinates of atom
- **mux,muy,muz** = components of dipole moment of atom (dipole units)
- **rho** = density (need units) for SPH particles
- **e** = energy (need units) for SPH particles
- **cv** = heat capacity (need units) for SPH particles
- **spin** = electron spin (+1/-1), 0 = nuclei, 2 = fixed-core, 3 = pseudo-cores (i.e. ECP)
- **eradius** = electron radius (or fixed-core radius)
- **etag** = integer ID of electron that each wavepacket belongs to
- **cs_re,cs_im** = real/imaginary parts of wavepacket coefficients

The units for these quantities depend on the unit style; see the units command for details.

For 2d simulations specify z as 0.0, or a value within the zlo zhi setting in the data file header.

The atom-ID is used to identify the atom throughout the simulation and in dump files. Normally, it is a unique value from 1 to Natoms for each atom. Unique values larger than Natoms can be used, but they will cause extra memory to be allocated on each processor, if an atom map array is used (see the atom_modify command). If an atom map array is not used (e.g. an atomic system with no bonds), and velocities are not assigned in the data file, and you don't care if unique atom IDs appear in dump files, then the atom-IDs can all be set to 0.

The molecule ID is a 2nd identifier attached to an atom. Normally, it is a number from 1 to N, identifying which molecule the atom belongs to. It can be 0 if it is an unbonded atom or if you don't care to keep track of molecule
assignments.

The diameter specifies the size of a finite-size spherical particle. It can be set to 0.0, which means that atom is a point particle.

The ellipsoidflag, lineflag, and triangleflag determine whether the particle is a finite-size ellipsoid or line or triangle of finite size, or a point particle. Additional attributes must be defined for each ellipsoid in the Ellipsoids section. Additional attributes must be defined for each line in the Lines section. Additional attributes must be defined for each triangle in the Triangles section.

Some pair styles and fixes and computes that operate on finite-size particles allow for a mixture of finite-size and point particles. See the doc pages of individual commands for details.

The density is used in conjunction with the particle volume for finite-size particles to set the mass of the particle as mass = density * volume. In this context, volume can be a 3d quantity (for spheres or ellipsoids), a 2d quantity (for triangles), or a 1d quantity (for line segments). If the volume is 0.0, meaning a point particle, then the density value is used as the mass.

For atom_style hybrid, following the 5 initial values (ID,type,x,y,z), specific values for each sub-style must be listed. The order of the sub-styles is the same as they were listed in the atom_style command. The sub-style specific values are those that are not the 5 standard ones (ID,type,x,y,z). For example, for the "charge" sub-style, a "q" value would appear. For the "full" sub-style, a "molecule-ID" and "q" would appear. These are listed in the same order they appear as listed above. Thus if

atom_style hybrid charge sphere

were used in the input script, each atom line would have these fields:

atom-ID atom-type x y z q diameter density

Note that if a non-standard value is defined by multiple sub-styles, it must appear multiple times in the atom line. E.g. the atom line for atom_style hybrid dipole full would list "q" twice:

atom-ID atom-type x y z q mux muy myz molecule-ID q

Atom lines (all lines or none of them) can optionally list 3 trailing integer values: nx,ny,nz. For periodic dimensions, they specify which image of the simulation box the atom is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as atoms cross periodic boundaries during the simulation. The flags can be output with atom snapshots via the dump command.

If nx,ny,nz values are not set in the data file, LAMMPS initializes them to 0. If image information is needed for later analysis and they are not all initially 0, it's important to set them correctly in the data file. Also, if you plan to use the replicate command to generate a larger system, these flags must be listed correctly for bonded atoms when the bond crosses a periodic boundary. I.e. the values of the image flags should be different by 1 (in the appropriate dimension) for the two atoms in such a bond.

Atom velocities and other atom quantities not defined above are set to 0.0 when the Atoms section is read. Velocities can be set later by a Velocities section in the data file or by a velocity or set command in the input script.

Bond Coeffs section:
one line per bond type
line syntax: ID coeffs

ID = bond type (1-N)
coeffs = list of coeffs

example:
4 250 1.49

The number and meaning of the coefficients are specific to the defined bond style. See the bond_style and bond_coeff commands for details. Coefficients can also be set via the bond_coeff command in the input script.

BondAngle Coeffs section:

one line per angle type
line syntax: ID coeffs

ID = angle type (1-N)
coeffs = list of coeffs (see class 2 section of angle_coeff)

BondBond Coeffs section:

one line per angle type
line syntax: ID coeffs

ID = angle type (1-N)
coeffs = list of coeffs (see class 2 section of angle_coeff)

BondBond13 Coeffs section:

one line per dihedral type
line syntax: ID coeffs

ID = dihedral type (1-N)
coeffs = list of coeffs (see class 2 section of dihedral_coeff)

Bonds section:

one line per bond
line syntax: ID type atom1 atom2

ID = bond number (1-Nbonds)
type = bond type (1-Nbondtype)
atom1,atom2 = IDs of 1st,2nd atoms in bond

example:
12 3 17 29

The Bonds section must appear after the Atoms section. All values in this section must be integers (1, not 1.0).

Dihedral Coeffs section:

one line per dihedral type
line syntax: ID coeffs
ID = dihedral type (1-N)
coeffs = list of coeffs

• example:

3 0.6 1 0 1

The number and meaning of the coefficients are specific to the defined dihedral style. See the dihedral_style and dihedral_coeff commands for details. Coefficients can also be set via the dihedral_coeff command in the input script.

Dihedrals section:

• one line per dihedral
• line syntax: ID type atom1 atom2 atom3 atom4

ID = number of dihedral (1-Ndihedrals)
type = dihedral type (1-Ndihedraltype)
atom1,atom2,atom3,atom4 = IDs of 1st,2nd,3rd,4th atoms in dihedral

• example:

12 4 17 29 30 21

The 4 atoms are ordered linearly within the dihedral. The Dihedrals section must appear after the Atoms section. All values in this section must be integers (1, not 1.0).

Ellipsoids section:

• one line per ellipsoid
• line syntax: atom-ID shapex shapey shapez quatw quati quatj quatk
• atom-ID = ID of atom which is an ellipsoid shapex,shapey,shapez = 3 diameters of ellipsoid (distance units) quatw,quati,quatj,quatk = quaternion components for orientation of atom example:

12 1 2 1 1 0 0 0

The Ellipsoids section must appear if atom_style ellipsoid is used and any atoms are listed in the Atoms section with an ellipsoidflag = 1. The number of ellipsoids should be specified in the header section via the "ellipsoids" keyword.

The 3 shape values specify the 3 diameters or aspect ratios of a finite-size ellipsoidal particle, when it is oriented along the 3 coordinate axes. They must all be non-zero values.

The values quatw, quati, quatj, and quatk set the orientation of the atom as a quaternion (4-vector). Note that the shape attributes specify the aspect ratios of an ellipsoidal particle, which is oriented by default with its x-axis along the simulation box's x-axis, and similarly for y and z. If this body is rotated (via the right-hand rule) by an angle theta around a unit vector (a,b,c), then the quaternion that represents its new orientation is given by (cos(theta/2), a*sin(theta/2), b*sin(theta/2), c*sin(theta/2)). These 4 components are quatw, quati, quatj, and quatk as specified above. LAMMPS normalizes each atom's quaternion in case (a,b,c) is not specified as a unit vector.

The Ellipsoids section must appear after the Atoms section.

EndBondTorsion Coeffs section:

• one line per dihedral type
• line syntax: ID coeffs
  
  `ID = dihedral type (1-N)`
  `coeffs = list of coeffs (see class 2 section of dihedral_coeff)`

**Improper Coeffs section:**

• one line per improper type
• line syntax: ID coeffs

  `ID = improper type (1-N)`
  `coeffs = list of coeffs`

• example:

  `2 20 0.0548311`

The number and meaning of the coefficients are specific to the defined improper style. See the `improper_style` and `improper_coeff` commands for details. Coefficients can also be set via the `improper_coeff` command in the input script.

**Impropers section:**

• one line per improper
• line syntax: ID type atom1 atom2 atom3 atom4

  `ID = number of improper (1-Nimpropers)`
  `type = improper type (1-Nimpropertype)`
  `atom1,atom2,atom3,atom4 = IDs of 1st,2nd,3rd,4th atoms in improper`

• example:

  `12 3 17 29 13 100`

The ordering of the 4 atoms determines the definition of the improper angle used in the formula for each improper style. See the doc pages for individual styles for details.

The **Impropers** section must appear after the **Atoms** section. All values in this section must be integers (1, not 1.0).

**Lines section:**

• one line per line segment
• line syntax: atom-ID x1 y1 x2 y2

• atom-ID = ID of atom which is a line segment x1,y1 = 1st end point x2,y2 = 2nd end point example:

  `12 1.0 0.0 2.0 0.0`

The **Lines** section must appear if `atom_style line` is used and any atoms are listed in the **Atoms** section with a lineflag = 1. The number of lines should be specified in the header section via the "lines" keyword.

The 2 end points are the end points of the line segment. The ordering of the 2 points should be such that using a right-hand rule to cross the line segment with a unit vector in the +z direction, gives an "outward" normal vector perpendicular to the line segment. I.e. normal = (c2-c1) x (0,0,1). This orientation may be important for defining some interactions.

The **Lines** section must appear after the **Atoms** section.
**Masses** section:

- one line per atom type
- line syntax: ID mass

  ID = atom type (1-N)
  mass = mass value

  example:

  3 1.01

This defines the mass of each atom type. This can also be set via the `mass` command in the input script. This section cannot be used for atom styles that define a mass for individual atoms - e.g. `atom_style sphere`.

**MiddleBondTorsion Coeffs** section:

- one line per dihedral type
- line syntax: ID coeffs

  ID = dihedral type (1-N)
  coeffs = list of coeffs (see class 2 section of `dihedral_coeff`)

**Pair Coeffs** section:

- one line per atom type
- line syntax: ID coeffs

  ID = atom type (1-N)
  coeffs = list of coeffs

  example:

  3 0.022 2.35197 0.022 2.35197

The number and meaning of the coefficients are specific to the defined pair style. See the `pair_style` and `pair_coeff` commands for details. Coefficients can also be set via the `pair_coeff` command in the input script.

**Triangles** section:

- one line per triangle
- line syntax: atom-ID x1 y1 x2 y2

  atom-ID = ID of atom which is a line segment x1,y1,z1 = 1st corner point x2,y2,z2 = 2nd corner point x3,y3,z3 = 3rd corner point

  example:

  12 0.0 0.0 0.0 2.0 0.0 1.0 0.0 0.0 2.0 1.0

The **Triangles** section must appear if `atom_style tri` is used and any atoms are listed in the *Atoms* section with a `triangleflag = 1`. The number of lines should be specified in the header section via the "triangles" keyword.

The 3 corner points are the corner points of the triangle. The ordering of the 3 points should be such that using a right-hand rule to go from point1 to point2 to point3 gives an "outward" normal vector to the face of the triangle. I.e. normal = (c2-c1) x (c3-c1). This orientation may be important for defining some interactions.
The **Triangles** section must appear after the **Atoms** section.

**Velocities section:**

- one line per atom
- line syntax: depends on atom style

<table>
<thead>
<tr>
<th>all styles except those listed</th>
<th>atom-ID vx vy vz</th>
</tr>
</thead>
<tbody>
<tr>
<td>dipole</td>
<td>atom-ID vx vy vz wx wy wz</td>
</tr>
<tr>
<td>electron</td>
<td>atom-ID vx vy vz ervel</td>
</tr>
<tr>
<td>ellipsoid</td>
<td>atom-ID vx vy vz lx ly lz</td>
</tr>
<tr>
<td>sphere</td>
<td>atom-ID vx vy vz wx wy wz</td>
</tr>
<tr>
<td>hybrid</td>
<td>atom-ID vx vy vz sub-style1 sub-style2 ...</td>
</tr>
</tbody>
</table>

where the keywords have these meanings:

vx, vy, vz = translational velocity of atom 
lx, ly, lz = angular momentum of aspherical atom 
xw, wy, wz = angular velocity of spherical atom 
ervel = electron radial velocity (0 for fixed-core): ul

The velocity lines can appear in any order. This section can only be used after an **Atoms** section. This is because the **Atoms** section must have assigned a unique atom ID to each atom so that velocities can be assigned to them.

Vx, vy, vz, and ervel are in units of velocity. Lx, ly, lz are in units of angular momentum (distance-velocity-mass). Wx, Wy, Wz are in units of angular velocity (radians/time).

For atom_style hybrid, following the 4 initial values (ID, vx, vy, vz), specific values for each sub-style must be listed. The order of the sub-styles is the same as they were listed in the **atom_style** command. The sub-style specific values are those that are not the 5 standard ones (ID, vx, vy, vz). For example, for the "sphere" sub-style, "wx", "wy", "wz" values would appear. These are listed in the same order they appear as listed above. Thus if

```plaintext
atom_style hybrid electron sphere
```

were used in the input script, each velocity line would have these fields:

```plaintext
atom-ID vx vy vz ervel wx wy wz
```

Note that if a non-standard value is defined by multiple sub-styles, it must appear multiple times in the velocity line. E.g. the velocity line for atom_style hybrid dipole sphere would list "wx" twice:

```plaintext
atom-ID vx vy vz wx wy wz wx wy wz
```

Translational velocities can also be set by the **velocity** command in the input script.

**Restrictions:**

To read gzipped data files, you must compile LAMMPS with the -DLAMMPS_GZIP option - see the **Making LAMMPS** section of the documentation.

**Related commands:**

read_dump, read_restart, create_atoms
Default: none
read_dump command

Syntax:

read_dump file Nstep field1 field2 ... keyword values ...

- file = name of dump file to read
- Nstep = snapshot timestep to read from file
- one or more fields may be appended

field = x or y or z or vx or vy or vz or ix or iy or iz
  x,y,z = atom coordinates
  vx,vy,vz = velocity components
  ix,iy,iz = image flags in each dimension

- zero or more keyword/value pairs may be appended
- keyword = box or replace or purge or trim or add or label or scaled or format

box value = yes or no = replace simulation box with dump box
replace value = yes or no = overwrite atoms with dump atoms
purge value = yes or no = delete all atoms before adding dump atoms
trim value = yes or no = trim atoms not in dump snapshot
add value = yes or no = add new dump atoms to system
label value = field column
  field = one of the listed fields or id or type
  column = label on corresponding column in dump file
scaled value = yes or no = coords in dump file are scaled/unscaled
format values = format of dump file, must be last keyword if used
  native = native LAMMPS dump file
  xyz = XYZ file
  molfile style path = VMD molfile plugin interface
  style = dcd or xyz or others supported by molfile
  path = optional path for location of molfile plugins

Examples:

read_dump dump.file 5000 x y z
read_dump dump.file 5000 x y vx vy trim yes
read_dump ../run7/dump.file.gz 10000 x y z box yes
read_dump dump.xyz 5 x y z box no format xyz
read_dump dump.xyz 10 x y z box no format molfile xyz ../plugins
read_dump dump.dcd 0 x y z box no format molfile dcd
read_dump dump.file 1000 x y z vx vy vz format molfile lammpstrj /usr/local/lib/vmd/plugins/LINUXAMD

Description:

Read atom information from a dump file to overwrite the current atom coordinates, and optionally the atom velocities and image flags and the simulation box dimensions. This is useful for restarting a run from a particular snapshot in a dump file. See the read_restart and read_data commands and the restart2data tool for alternative methods to do this. Also see the rerun command for a means of reading multiple snapshots from a dump file.

Note that a simulation box must already be defined before using the read_dump command. This can be done by the create_box, read_data, or read_restart commands. The read_dump command can reset the simulation box dimensions, as explained below.
Also note that reading per-atom information from a dump snapshot is limited to the atom coordinates, velocities and image flags, as explained below. Other atom properties, which may be necessary to run a valid simulation, such as atom charge, or bond topology information for a molecular system, are not read from (or even contained in) dump files. Thus this auxiliary information should be defined in the usual way, e.g. in a data file read in by a read_data command, before using the read_dump command, or by the set command, after the dump snapshot is read.

If the dump filename specified as file ends with ".gz", the dump file is read in gzipped format. You cannot (yet) read a dump file that was written in binary format with a "bin" suffix, or to multiple files via the "%" option in the dump file name. See the dump command for details.

The format of the dump file is selected through the format keyword. If specified, it must be the last keyword used, since all remaining arguments are passed on to the dump reader. The native format is for native LAMMPS dump files, written with a "dump atom".html or dump custom command. The xyz format is for generic XYZ formatted dump files.

The molfile format supports reading data through using the VMD molfile plugin interface. This dump reader format is only available, if the USER-MOLFILE package has been installed when compiling LAMMPS.

The molfile format takes one or two additional values. The style value determines the file format to be used and can be any format that the molfile plugins support, such as DCD or XYZ. Note that DCD dump files can be written by LAMMPS via the dump dcd command. The path value specifies a list of directories which LAMMPS will search for the molfile plugins appropriate to the specified style. The syntax of the path value is like other search paths: it can contain multiple directories separated by a colon (or semi-colon on windows). The path keyword is optional and defaults to ".", i.e. the current directory.

Support for other dump format readers may be added in the future.

Global information is first read from the dump file, namely timestep and box information.

The dump file is scanned for a snapshot with a time stamp that matches the specified Nstep. This means the LAMMPS timestep the dump file snapshot was written on for the native format. However, the xyz and molfile formats do not store the timestep. For these formats, timesteps are numbered logically, in a sequential manner, starting from 0. Thus to access the 10th snapshot in an xyz or molfile formatted dump file, use Nstep = 9.

The dimensions of the simulation box for the selected snapshot are also read; see the box keyword discussion below. For the native format, an error is generated if the snapshot is for a triclinic box and the current simulation box is orthogonal or vice versa. A warning will be generated if the snapshot box boundary conditions (periodic, shrink-wrapped, etc) do not match the current simulation boundary conditions, but the boundary condition information in the snapshot is otherwise ignored. See the "boundary" command for more details.

For the xyz format, no information about the box is available, so you must set the box flag to no. See details below.

For the molfile format, reading simulation box information is typically supported, but the location of the simulation box origin is lost and no explicit information about periodicity or orthogonal/triclinic box shape is available. The USER-MOLFILE package makes a best effort to guess based on heuristics, but this may not always work perfectly.

Per-atom information from the dump file snapshot is then read from the dump file snapshot. This corresponds to the specified fields listed in the read_dump command. It is an error to specify a z-dimension field, namely z, vz, or iz, for a 2d simulation.
For dump files in *native* format, each column of per-atom data has a text label listed in the file. A matching label for each field must appear, e.g. the label "vy" for the field vy. For the x, y, z fields any of the following labels are considered a match:

- x, xs, xu, xsu for field x
- y, ys, yu, ysu for field y
- z, zs, zu, zsu for field z

The meaning of xs (scaled), xu (unwrapped), and xsu (scaled and unwrapped) is explained on the dump command doc page. These labels are searched for in the list of column labels in the dump file, in order, until a match is found.

The dump file must also contain atom IDs, with a column label of "id".

If the *add* keyword is specified with a value of *yes*, as discussed below, the dump file must contain atom types, with a column label of "type".

If a column label in the dump file is not a match to a specified field, the *label* keyword can be used to specify which column label to associate with that field. An example is if a time-averaged coordinate is written to the dump file via the fix ave/atom command. The column will then have a label corresponding to the fix-ID rather than "x" or "xs". The *label* keyword can also be used to specify new column labels for fields *id* and *type*.

For dump files in *xyz* format, only the x, y, and z fields are supported. The dump file does not store atom IDs, so these are assigned consecutively to the atoms as they appear in the dump file, starting from 1. Thus you should insure that order of atoms is consistent from snapshot to snapshot in the the XYZ dump file. See the dump_modify sort command if the XYZ dump file was written by LAMMPS.

For dump files in *molfile* format, the x, y, z, vx, vy, and vz fields can be specified. However, not all molfile formats store velocities, or their respective plugins may not support reading of velocities. The molfile dump files do not store atom IDs, so these are assigned consecutively to the atoms as they appear in the dump file, starting from 1. Thus you should insure that order of atoms are consistent from snapshot to snapshot in the the molfile dump file. See the dump_modify sort command if the dump file was written by LAMMPS.

Information from the dump file snapshot is used to overwrite or replace properties of the current system. There are various options for how this is done, determined by the specified fields and optional keywords.

The timestep of the snapshot becomes the current timestep for the simulation. See the *reset_timestep* command if you wish to change this after the dump snapshot is read.

If the *box* keyword is specified with a *yes* value, then the current simulation box dimensions are replaced by the dump snapshot box dimensions. If the *box* keyword is specified with a *no* value, the current simulation box is unchanged.

If the *purge* keyword is specified with a *yes* value, then all current atoms in the system are deleted before any of the operations invoked by the replace, trim, or add keywords take place.

If the *replace* keyword is specified with a *yes* value, then atoms with IDs that are in both the current system and the dump snapshot have their properties overwritten by field values. If the *replace* keyword is specified with a *no* value, atoms with IDs that are in both the current system and the dump snapshot are not modified.

If the *trim* keyword is specified with a *yes* value, then atoms with IDs that are in the current system but not in the dump snapshot are deleted. These atoms are unaffected if the *trim* keyword is specified with a *no* value.
If the *add* keyword is specified with a *yes* value, then atoms with IDs that are in the dump snapshot, but not in the current system are added to the system. These dump atoms are ignored if the *add* keyword is specified with a *no* value.

Note that atoms added via the *add* keyword will have only the attributes read from the dump file due to the *field* arguments. If \(x\) or \(y\) or \(z\) is not specified as a field, a value of 0.0 is used for added atoms. Added atoms must have an atom type, so this value must appear in the dump file.

Any other attributes (e.g. charge or particle diameter for spherical particles) will be set to default values, the same as if the *create_atoms* command were used.

Note that atom IDs are not preserved for new dump snapshot atoms added via the *add* keyword. The procedure for assigning new atom IDs to added atoms is the same as described for the *create_atoms* command.

Atom coordinates read from the dump file are converted into absolute, unscaled coordinates, relative to the box dimensions of the snapshot. These coordinates may then be assigned to an existing or new atom in the current simulation. The coordinates will be remapped to the simulation box, whether it is the original box or the dump snapshot box. If periodic boundary conditions apply, this means the atom will be remapped back into the box if necessary. If shrink-wrap boundary conditions apply, the new coordinates may change the current box dimensions. If fixed boundary conditions apply, the atom will be lost if it is outside the simulation box.

For *native* format dump files, the 3 \(xyz\) image flags for an atom in the dump file are set to the corresponding values appearing in the dump file if the \(ix\), \(iy\), \(iz\) fields are specified. If not specified, the image flags for replaced atoms are not changed and image flags for new atoms are set to default values. The remapping procedure described in the previous paragraph can change image flags for all atoms (old and new) if periodic boundary conditions are applied to remap an atom back into the simulation box. Note that inconsistent image flag values can result if you use image flag fields from the dump file but do not also use the dump file box parameters.

LAMMPS knows how to compute absolute, unscaled coordinates for the snapshot column labels discussed above, e.g. \(x\), \(xs\), \(xu\), \(xsu\). If another column label is assigned to the \(x\) or \(y\) or \(z\) field via the *label* keyword, e.g. for coordinates output by the *fix ave/atom* command, then LAMMPS needs to know whether the coordinate information in the dump file is scaled or unscaled. This can be set via the *scaled* keyword. The value of the *scaled* keyword is ignored for field \(x\) or \(y\) or \(z\) if the *label* keyword is not used to assign a column label to that field.

The scaled vs unscaled setting must be consistent for any of the \(x\), \(y\), \(z\) fields that are specified. If the dump file coordinates are scaled and the simulation box is triclinic, then all 3 of the \(x\), \(y\), \(z\) fields must be specified, since they are all needed to generate absolute, unscaled coordinates.

**Restrictions:**

To read gzipped dump files, you must compile LAMMPS with the -DLAMMPS_GZIP option - see the Making LAMMPS section of the documentation.

The *molfile* dump file formats are part of the USER-MOLFILE package. They are only enabled if LAMMPS was built with that packages. See the Making LAMMPS section for more info.

**Related commands:**

dump, dump molfile, read_data, read_restart, rerun

**Default:**
The option defaults are box = yes, replace = yes, purge = no, trim = no, add = no, scaled = no, and format = native.
read_restart command

Syntax:

```
read_restart file
```

- file = name of binary restart file to read in

Examples:

```
read_restart save.10000
read_restart restart.*
read_restart poly.*.%
```

Description:

Read in a previously saved simulation from a restart file. This allows continuation of a previous run. Information about what is stored in a restart file is given below.

Restart files are saved in binary format to enable exact restarts, meaning that the trajectories of a restarted run will precisely match those produced by the original run had it continued on.

Several things can prevent exact restarts due to round-off effects, in which case the trajectories in the 2 runs will slowly diverge. These include running on a different number of processors or changing certain settings such as those set by the newton or processors commands. LAMMPS will issue a warning in these cases.

Certain fixes will not restart exactly, though they should provide statistically similar results. These include fix shake and fix langevin.

Certain pair styles will not restart exactly, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities, which are used at half-step values every timestep when forces are computed. When a run restarts, forces are initially evaluated with a full-step velocity, which is different than if the run had continued. These pair styles include granular pair styles, pair dpd, and pair lubricate.

If a restarted run is immediately different than the run which produced the restart file, it could be a LAMMPS bug, so consider reporting it if you think the behavior is wrong.

Because restart files are binary, they may not be portable to other machines. They can be converted to ASCII data files using the restart2data tool in the tools sub-directory of the LAMMPS distribution.

Similar to how restart files are written (see the write_restart and restart commands), the restart filename can contain two wild-card characters. If a "*" appears in the filename, the directory is searched for all filenames that match the pattern where "*" is replaced with a timestep value. The file with the largest timestep value is read in. Thus, this effectively means, read the latest restart file. It's useful if you want your script to continue a run from where it left off. See the run command and its "upto" option for how to specify the run command so it doesn't need to be changed either.

If a "%" character appears in the restart filename, LAMMPS expects a set of multiple files to exist. The restart and write_restart commands explain how such sets are created. Read_restart will first read a filename where "%" is replaced by "base". This file tells LAMMPS how many processors created the set. Read_restart then reads the
additional files. For example, if the restart file was specified as save.% when it was written, then read_restart reads the files save.base, save.0, save.1, ... save.P-1, where P is the number of processors that created the restart file. The processors in the current LAMMPS simulation share the work of reading these files; each reads a roughly equal subset of the files. The number of processors which created the set can be different the number of processors in the current LAMMPS simulation. This can be a fast mode of input on parallel machines that support parallel I/O.

A restart file stores the following information about a simulation: units and atom style, simulation box size and shape and boundary settings, group definitions, per-type atom settings such as mass, per-atom attributes including their group assignments and molecular topology attributes, force field styles and coefficients, and special_bonds settings. This means that commands for these quantities do not need to be re-specified in the input script that reads the restart file, though you can redefine settings after the restart file is read.

One exception is that some pair styles do not store their info in restart files. The doc pages for individual pair styles note if this is the case. This is also true of bond_style hybrid (and angle_style, dihedral_style, improper_style hybrid).

Information about kspace_style settings are not stored in the restart file. Hence if you wish to use an Ewald or PPPM solver, these commands must be re-issued after the restart file is read.

The list of fixes used for a simulation is not stored in the restart file. This means the new input script should specify all fixes it will use. Note that some fixes store an internal "state" which is written to the restart file. This allows the fix to continue on with its calculations in a restarted simulation. To re-enable such a fix, the fix command in the new input script must use the same fix-ID and group-ID as was used in the input script that wrote the restart file. If a match is found, LAMMPS prints a message indicating that the fix is being re-enabled. If no match is found before the first run or minimization is performed by the new script, the "state" information for the saved fix is discarded. See the doc pages for individual fixes for info on which ones can be restarted in this manner.

Bond interactions (angle, etc) that have been turned off by the fix shake or delete_bonds command will be written to a restart file as if they are turned on. This means they will need to be turned off again in a new run after the restart file is read.

Bonds that are broken (e.g. by a bond-breaking potential) are written to the restart file as broken bonds with a type of 0. Thus these bonds will still be broken when the restart file is read.

IMPORTANT NOTE: No other information is stored in the restart file. This means that an input script that reads a restart file should specify settings for quantities like timestep size, thermodynamic, neighbor list criteria including settings made via the neigh_modify comand, dump file output, geometric regions, etc.

Restrictions: none

Related commands:
read_data, read_dump, write_restart, restart

Default: none
region command

Syntax:

region ID style args keyword arg ... 

- ID = user-assigned name for the region
- style = delete or block or cone or cylinder or plane or prism or sphere or union or intersect

delete = no args
block args = xlo xhi ylo yhi zlo zhi
  xlo, xhi, ylo, yhi, zlo, zhi = bounds of block in all dimensions (distance units)
cone args = dim c1 c2 radlo radhi lo hi
  dim = x or y or z = axis of cone
  c1, c2 = coords of cone axis in other 2 dimensions (distance units)
  radlo, radhi = cone radii at lo and hi end (distance units)
  lo, hi = bounds of cone in dim (distance units)
cylinder args = dim c1 c2 radius lo hi
  dim = x or y or z = axis of cylinder
  c1, c2 = coords of cylinder axis in other 2 dimensions (distance units)
  radius = cylinder radius (distance units)
  lo, hi = bounds of cylinder in dim (distance units)
plane args = px py pz nx ny nz
  px, py, pz = point on the plane (distance units)
  nx, ny, nz = direction normal to plane (distance units)
prism args = xlo xhi ylo yhi zlo zhi xy xz yz
  xlo, xhi, ylo, yhi, zlo, zhi = bounds of untitled prism (distance units)
  xy = distance to tilt y in x direction (distance units)
  xz = distance to tilt z in x direction (distance units)
  yz = distance to tilt z in y direction (distance units)
sphere args = x y z radius
  x, y, z = center of sphere (distance units)
  radius = radius of sphere (distance units)
union args = N reg-ID1 reg-ID2 ...
  N = # of regions to follow, must be 2 or greater
  reg-ID1, reg-ID2, ... = IDs of regions to join together
intersect args = N reg-ID1 reg-ID2 ...
  N = # of regions to follow, must be 2 or greater
  reg-ID1, reg-ID2, ... = IDs of regions to intersect

- zero or more keyword/arg pairs may be appended
- keyword = side or units or move or rotate

side value = in or out
  in = the region is inside the specified geometry
  out = the region is outside the specified geometry
units value = lattice or box
  lattice = the geometry is defined in lattice units
  box = the geometry is defined in simulation box units
move args = v_x v_y v_z
  v_x, v_y, v_z = equal-style variables for x, y, z displacement of region over time
rotate args = v_theta Px Py Pz Rx Ry Rz
  v_theta = equal-style variable for rotation of region over time (in radians)
  Px, Py, Pz = origin for axis of rotation (distance units)
  Rx, Ry, Rz = axis of rotation vector

Examples:

region 1 block -3.0 5.0 INF 10.0 INF INF
Description:

This command defines a geometric region of space. Various other commands use regions. For example, the region can be filled with atoms via the `create_atoms` command. Or a bounding box around the region, can be used to define the simulation box via the `create_box` command. Or the atoms in the region can be identified as a group via the `group` command, or deleted via the `delete_atoms` command. Or the surface of the region can be used as a boundary wall via the `fix wall/region` command.

Commands which use regions typically test whether an atom's position is contained in the region or not. For this purpose, coordinates exactly on the region boundary are considered to be interior to the region. This means, for example, for a spherical region, an atom on the sphere surface would be part of the region if the sphere were defined with the `side in` keyword, but would not be part of the region if it were defined using the `side out` keyword. See more details on the `side` keyword below.

Normally, regions in LAMMPS are "static", meaning their geometric extent does not change with time. If the `move` or `rotate` keyword is used, as described below, the region becomes "dynamic", meaning it's location or orientation changes with time. This may be useful, for example, when thermostating a region, via the compute temp/region command, or when the fix wall/region command uses a region surface as a bounding wall on particle motion, i.e. a rotating container.

The `delete` style removes the named region. Since there is little overhead to defining extra regions, there is normally no need to do this, unless you are defining and discarding large numbers of regions in your input script.

The lo/hi values for `block` or `cone` or `cylinder` or `prism` styles can be specified as EDGE or INF. EDGE means they extend all the way to the global simulation box boundary. Note that this is the current box boundary; if the box changes size during a simulation, the region does not. INF means a large negative or positive number (1.0e20), so it should encompass the simulation box even if it changes size. If a region is defined before the simulation box has been created (via create_box or read_data or read_restart commands), then an EDGE or INF parameter cannot be used. For a `prism` region, a non-zero tilt factor in any pair of dimensions cannot be used if both the lo/hi values in either of those dimensions are INF. E.g. if the xy tilt is non-zero, then xlo and xhi cannot both be INF, nor can ylo and yhi.

IMPORTANT NOTE: Regions in LAMMPS do not get wrapped across periodic boundaries, as specified by the `boundary` command. For example, a spherical region that is defined so that it overlaps a periodic boundary is not treated as 2 half-spheres, one on either side of the simulation box.

IMPORTANT NOTE: Regions in LAMMPS are always 3d geometric objects, regardless of whether the dimension of a simulation is 2d or 3d. Thus when using regions in a 2d simulation, you should be careful to define the region so that its intersection with the 2d x-y plane of the simulation has the 2d geometric extent you want.

For style `cone`, an axis-aligned cone is defined which is like a `cylinder` except that two different radii (one at each end) can be defined. Either of the radii (but not both) can be 0.0.

For style `cone` and `cylinder`, the c1,c2 params are coordinates in the 2 other dimensions besides the cylinder axis dimension. For dim = x, c1/c2 = y/z; for dim = y, c1/c2 = x/z; for dim = z, c1/c2 = x/y. Thus the third example above specifies a cylinder with its axis in the y-direction located at x = 2.0 and z = 3.0, with a radius of 5.0, and extending in the y-direction from -5.0 to the upper box boundary.
For style *plane*, a plane is defined which contain the point \((px,py,pz)\) and has a normal vector \((nx,ny,nz)\). The normal vector does not have to be of unit length. The "inside" of the plane is the half-space in the direction of the normal vector; see the discussion of the *side* option below.

For style *prism*, a parallelepiped is defined (it's too hard to spell parallelepiped in an input script!). The parallelepiped has its "origin" at \((xlo,ylo,zlo)\) and is defined by 3 edge vectors starting from the origin given by \(A = (xhi-xlo,0,0); B = (xy,yhi-ylo,0); C = (xz,yz,zhi-zlo)\). \(Xy,xz,yz\) can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped.

A prism region that will be used with the *create_box* command to define a triclinic simulation box must have tilt factors \((xy,xz,yz)\) that do not skew the box more than half the distance of corresponding the parallel box length. For example, if \(xlo = 2\) and \(xhi = 12\), then the \(x\) box length is 10 and the \(xy\) tilt factor must be between -5 and 5. Similarly, both \(xz\) and \(yz\) must be between \(-(xhi-xlo)/2\) and \(+(yhi-ylo)/2\). Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all geometrically equivalent.

See Section *howto 12* of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

The *union* style creates a region consisting of the volume of all the listed regions combined. The *intersect* style creates a region consisting of the volume that is common to all the listed regions.

The *side* keyword determines whether the region is considered to be inside or outside of the specified geometry. Using this keyword in conjunction with *union* and *intersect* regions, complex geometries can be built up. For example, if the interior of two spheres were each defined as regions, and a *union* style with *side* = out was constructed listing the region-IDs of the 2 spheres, the resulting region would be all the volume in the simulation box that was outside both of the spheres.

The *units* keyword determines the meaning of the distance units used to define the region for any argument above listed as having distance units. It also affects the scaling of the velocity vector specified with the *vel* keyword, the amplitude vector specified with the *wiggle* keyword, and the rotation point specified with the *rotate* keyword, since they each involve a distance metric.

A *box* value selects standard distance units as defined by the *units* command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The *lattice* command must have been previously used to define the lattice spacings which are used as follows:

- For style *block*, the lattice spacing in dimension \(x\) is applied to \(xlo\) and \(xhi\), similarly the spacings in dimensions \(y,z\) are applied to \(ylo/yhi\) and \(zlo/zhi\).
- For style *cone*, the lattice spacing in argument *dim* is applied to \(lo\) and \(hi\). The spacings in the two radial dimensions are applied to \(c1\) and \(c2\). The two cone radii are scaled by the lattice spacing in the dimension corresponding to \(c1\).
- For style *cylinder*, the lattice spacing in argument *dim* is applied to \(lo\) and \(hi\). The spacings in the two radial dimensions are applied to \(c1\) and \(c2\). The cylinder radius is scaled by the lattice spacing in the dimension corresponding to \(c1\).
- For style *plane*, the lattice spacing in dimension \(x\) is applied to \(px\) and \(nx\), similarly the spacings in dimensions \(y,z\) are applied to \(py/ny\) and \(pz/nz\).
- For style *prism*, the lattice spacing in dimension \(x\) is applied to \(xlo\) and \(xhi\), similarly for \(ylo/yhi\) and \(zlo/zhi\). The lattice spacing in dimension \(x\) is applied to \(xy\) and \(xz\), and the spacing in dimension \(y\) to \(yz\).
- For style *sphere*, the lattice spacing in dimensions \(x,y,z\) are applied to the sphere center \(x,y,z\). The spacing in dimension \(x\) is applied to the sphere radius.
If the *move* or *rotate* keywords are used, the region is "dynamic", meaning its location or orientation changes with time. These keywords cannot be used with a *union* or *intersect* style region. Instead, the keywords should be used to make the individual sub-regions of the *union* or *intersect* region dynamic. Normally, each sub-region should be "dynamic" in the same manner (e.g. rotate around the same point), though this is not a requirement.

The *move* keyword allows one or more equal-style variables to be used to specify the x,y,z displacement of the region, typically as a function of time. A variable is specified as v_name, where name is the variable name. Any of the three variables can be specified as NULL, in which case no displacement is calculated in that dimension.

Note that equal-style variables can specify formulas with various mathematical functions, and include *thermo_style* command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a region displacement that change as a function of time or spans consecutive runs in a continuous fashion. For the latter, see the *start* and *stop* keywords of the *run* command and the *elaplong* keyword of *thermo_style custom* for details.

For example, these commands would displace a region from its initial position, in the positive x direction, effectively at a constant velocity:

```plaintext
variable dx equal ramp(0,10)
region 2 sphere 10.0 10.0 0.0 5 move v_dx NULL NULL
```

Note that the initial displacement is 0.0, though that is not required.

Either of these variables would "wiggle" the region back and forth in the y direction:

```plaintext
variable dy equal swiggle(0,5,100)
variable dysame equal 5*sin(2*PI*elaplong*dt/100)
region 2 sphere 10.0 10.0 0.0 5 move NULL v_dy NULL
```

The *rotate* keyword rotates the region around a rotation axis \( R = (Rx,Ry,Rz) \) that goes thru a point \( P = (Px,Py,Pz) \). The rotation angle is calculated, presumably as a function of time, by a variable specified as v_theta, where theta is the variable name. The variable should generate its result in radians. The direction of rotation for the region around the rotation axis is consistent with the right-hand rule: if your right-hand thumb points along \( R \), then your fingers wrap around the axis in the direction of rotation.

The *move* and *rotate* keywords can be used together. In this case, the displacement specified by the *move* keyword is applied to the \( P \) point of the *rotate* keyword.

**Restrictions:**

A prism cannot be of 0.0 thickness in any dimension; use a small z thickness for 2d simulations. For 2d simulations, the \( xz \) and \( yz \) parameters must be 0.0.

**Related commands:**

*lattice*, *create_atoms*, *delete_atoms*, *group*

**Default:**

The option defaults are *side = in*, *units = lattice*, and *no move or rotation*. 
replicate command

Syntax:

replicate nx ny nz

• nx,ny,nz = replication factors in each dimension

Examples:

replicate 2 3 2

Description:

Replicate the current simulation one or more times in each dimension. For example, replication factors of 2,2,2 will create a simulation with 8x as many atoms by doubling the simulation domain in each dimension. A replication factor of 1 in a dimension leaves the simulation domain unchanged.

All properties of the atoms are replicated, including their velocities, which may or may not be desirable. New atom IDs are assigned to new atoms, as are molecule IDs. Bonds and other topology interactions are created between pairs of new atoms as well as between old and new atoms. This is done by using the image flag for each atom to "unwrap" it out of the periodic box before replicating it. This means that molecular bonds you specify in the original data file that span the periodic box should be between two atoms with image flags that differ by 1. This will allow them to be unwrapped appropriately.

Restrictions:

A 2d simulation cannot be replicated in the z dimension.

If a simulation is non-periodic in a dimension, care should be used when replicating it in that dimension, as it may put atoms nearly on top of each other.

If the current simulation was read in from a restart file (before a run is performed), there can have been no fix information stored in the file for individual atoms. Similarly, no fixes can be defined at the time the replicate command is used that require vectors of atom information to be stored. This is because the replicate command does not know how to replicate that information for new atoms it creates.

Replicating a system that has rigid bodies (defined via the fix rigid command), either currently defined or that created the restart file which was read in before replicating, can cause problems if there is a bond between a pair of rigid bodies that straddle a periodic boundary. This is because the periodic image information for particles in the rigid bodies are set differently than for a non-rigid system and can result in a new bond being created that spans the periodic box. Thus you cannot use the replicate command in this scenario.

Related commands: none

Default: none
rerun command

Syntax:

rerun file1 file2 ... keyword args ...

- file1,file2,... = dump file(s) to read
- one or more keywords may be appended, keyword *dump* must appear and be last

keyword = *first* or *last* or *every* or *skip* or *start* or *stop* or *dump*

first args = Nfirst
  Nfirst = dump timestep to start on

last args = Nlast
  Nlast = dump timestep to stop on

every args = Nevery
  Nevery = read snapshots matching every this many timesteps

skip args = Nskip
  Nskip = read one out of every Nskip snapshots

start args = Nstart
  Nstart = timestep on which pseudo run will start

stop args = Nstop
  Nstop = timestep to which pseudo run will end

dump args = same as read_dump command starting with its field arguments

Examples:

rerun dump.file dump x y z vx vy vz
rerun dump1.txt dump2.txt first 10000 every 1000 dump x y z
rerun dump.vels dump x y z vx vy vz box yes format molfile lammpstrj
rerun dump.dcd dump x y z box no format molfile dcd
rerun ../run7/dump.file.gz skip 2 dump x y z box yes

Description:

Perform a pseudo simulation run where atom information is read one snapshot at a time from a dump file(s), and energies and forces are computed on the snapshot to produce thermodynamic or other output.

This can be useful in the following kinds of scenarios, after an initial simulation produced the dump file:

- Compute the energy and forces of snapshots using a different potential.
- Calculate one or more diagnostic quantities on the snapshots that weren't computed in the initial run. These can also be computed with settings not used in the initial run, e.g. computing an RDF via the compute rdf command with a longer cutoff than was used initially.
- Calculate the portion of per-atom forces resulting from a subset of the potential. E.g. compute only Coulombic forces. This can be done by only defining only a Coulombic pair style in the rerun script. Doing this in the original script would result in different (bad) dynamics.

Conceptually, using the rerun command is like running an input script that has a loop in it (see the next and jump commands). Each iteration of the loop reads one snapshot from the dump file via the read_dump command, sets the timestep to the appropriate value, and then invokes a run command for zero timesteps to simply compute energy and forces, and any other thermodynamic output or diagnostic info you have defined. This computation also invokes any fixes you have defined that apply constraints to the system, such as fix shake or fix indent.
Note that a simulation box must already be defined before using the rerun command. This can be done by the create_box, read_data, or read_restart commands.

Also note that reading per-atom information from dump snapshots is limited to the atom coordinates, velocities and image flags as explained in the read_dump command. Other atom properties, which may be necessary to compute energies and forces, such as atom charge, or bond topology information for a molecular system, are not read from (or even contained in) dump files. Thus this auxiliary information should be defined in the usual way, e.g. in a data file read in by a read_data command, before using the rerun command.

If more than one dump file is specified, the dump files are read one after the other. It is assumed that snapshot timesteps will be in ascending order. If a snapshot is encountered that is not in ascending order, it will cause the rerun command to complete.

The first, last, every, skip keywords determine which snapshots are read from the dump file(s). Snapshots are skipped until they have a timestamp >= Nfirst. When a snapshot with a timestamp > Nlast is encountered, the rerun command finishes. Note below that the defaults for first and last are to read all snapshots. If the every keyword is set to a value > 0, then only snapshots with timestamps that are a multiple of Nevery are read (the first snapshot is always read). If Nevery = 0, then this criterion is ignored, i.e. every snapshot is read that meets the other criteria. If the skip keyword is used, then after the first snapshot is read, every Nth snapshot is read, where N = Nskip. E.g. if Nskip = 3, then only 1 out of every 3 snapshots is read, assuming the snapshot timestamp is also consistent with the other criteria.

The start and stop keywords have the same meaning that they do for the run command. They only need to be defined if (a) you are using a fix command that changes some value over time, and (b) you want the reference point for elapsed time (from start to stop) to be different than the first and last settings. See the doc page for individual fixes to see which ones can be used with the start/stop keywords. Note that if you define neither of the start/stop or first/last keywords, then LAMMPS treats the pseudo run as going from 0 to a huge value (effectively infinity). This means that any quantity that a fix scales as a fraction of elapsed time in the run, will essentially remain at its initial value.

The dump keyword is required and must be the last keyword specified. Its arguments are passed internally to the read_dump command. See the read_dump doc page for details on the various options it allows for extracting information from the dump file snapshots, and for using that information to alter the LAMMPS simulation.

In general, a LAMMPS input script that uses a rerun command can include and perform all the usual operations of an input script that uses the run command. There are a few exceptions and points to consider, as discussed here.

Fixes that perform time integration, such as fix nve or fix npt are not invoked, since no time integration is performed. Fixes that perturb or constrain the forces on atoms will be invoked, just as they would during a normal run. Examples are fix indent and fix langevin. So you should think carefully as to whether that makes sense for the manner in which you are reprocessing the dump snapshots.

If you only want the rerun script to perform analyses that do not involve pair interactions, such as use compute msd to calculated displacements over time, you do not need to define a pair style, which may also mean neighbor lists will not need to be calculated which saves time. The communicate cutoff command can also be used to insure ghost atoms are acquired from far enough away for operations like bond and angle evaluations, if no pair style is being used.

Every time a snapshot is read, the timestep for the simulation is reset, as if the >reset_timestep command were used. This command has some restrictions as to what fixes can be defined. See its doc page for details. For example, the fix deposit and fix dt/reset fixes are in this category. They also make no sense to use with a rerun
command.

If time-averaging fixes like `fix ave/time` are used, they are invoked on timesteps that are a function of their `Nevery`, `Nrepeat`, and `Nfreq` settings. As an example, see the `fix ave/time` doc page for details. You must insure those settings are consistent with the snapshot timestamps that are read from the dump file(s). If an averaging fix is not invoked on a timestep it expects to be, LAMMPS will flag an error.

The various forms of LAMMPS output, as defined by the `thermo_style`, `thermo`, `dump`, and `restart` commands occur on specific timesteps. If successive dump snapshots skip those timesteps, then no output will be produced. E.g. if you request thermodynamic output every 100 steps, but the dump file snapshots are every 1000 steps, then you will only see thermodynamic output every 1000 steps.

**Restrictions:**

To read gzipped dump files, you must compile LAMMPS with the `-DLAMMPS_GZIP` option - see the Making LAMMPS section of the documentation.

**Related commands:**

`read_dump`

**Default:**

The option defaults are first = 0, last = a huge value (effectively infinity), start = same as first, stop = same as last, every = 0, skip = 1;
reset_timestep command

Syntax:

reset_timestep N

- N = timestep number

Examples:

reset_timestep 0
reset_timestep 4000000

Description:

Set the timestep counter to the specified value. This command normally comes after the timestep has been set by reading a restart file via the read_restart command, or a previous simulation advanced the timestep.

The read_data and create_box commands set the timestep to 0; the read_restart command sets the timestep to the value it had when the restart file was written.

Restrictions: none

This command cannot be used when any fixes are defined that keep track of elapsed time to perform certain kinds of time-dependent operations. Examples are the fix deposit and fix dt/reset commands. The former adds atoms on specific timesteps. The latter keeps track of accumulated time.

Various fixes use the current timestep to calculate related quantities. If the timestep is reset, this may produce unexpected behavior, but LAMMPS allows the fixes to be defined even if the timestep is reset. For example, commands which thermostat the system, e.g. fix nvt, allow you to specify a target temperature which ramps from Tstart to Tstop which may persist over several runs. If you change the timestep, you may induce an instantaneous change in the target temperature.

Resetting the timestep clears flags for computes that may have calculated some quantity from a previous run. This means these quantity cannot be accessed by a variable in between runs until a new run is performed. See the variable command for more details.

Related commands:

rerun

Default: none
restart command

Syntax:

restart 0
restart N root
restart N file1 file2

- N = write a restart file every this many timesteps
- N can be a variable (see below)
- root = filename to which timestep # is appended
- file1, file2 = two full filenames, toggle between them when writing file

Examples:

restart 0
restart 1000 poly.restart
restart 1000 restart.*.equil
restart 10000 poly.%1 poly.%2
restart v_mystep poly.restart

Description:

Write out a binary restart file every so many timesteps, in either or both of two modes, as a run proceeds. A value of 0 means do not write out any restart files. The two modes are as follows. If one filename is specified, a series of filenames will be created which include the timestep in the filename. If two filenames are specified, only 2 restart files will be created, with those names. LAMMPS will toggle between the 2 names as it writes successive restart files.

Note that you can specify the restart command twice, once with a single filename and once with two filenames. This would allow you, for example, to write out archival restart files every 100000 steps using a single filename, and more frequent temporary restart files every 1000 steps, using two filenames. Using restart 0 will turn off both modes of output.

Similar to dump files, the restart filename(s) can contain two wild-card characters.

If a "*" appears in the single filename, it is replaced with the current timestep value. This is only recognized when a single filename is used (not when toggling back and forth). Thus, the 3rd example above creates restart files as follows: restart.1000.equil, restart.2000.equil, etc. If a single filename is used with no "*", then the timestep value is appended. E.g. the 2nd example above creates restart files as follows: poly.restart.1000, poly.restart.2000, etc.

If a "%" character appears in the restart filename(s), then one file is written for each processor and the "%" character is replaced with the processor ID from 0 to P-1. An additional file with the "%" replaced by "base" is also written, which contains global information. For example, the files written on step 1000 for filename restart.% would be restart.base.1000, restart.0.1000, restart.1.1000, ..., restart.P-1.1000. This creates smaller files and can be a fast mode of output and subsequent input on parallel machines that support parallel I/O.

Restart files are written on timesteps that are a multiple of N but not on the first timestep of a run or minimization. You can use the write_restart command to write a restart file before a run begins. A restart file is not written on the last timestep of a run unless it is a multiple of N. A restart file is written on the last timestep of a minimization if N > 0 and the minimization converges.
Instead of a numeric value, N can be specified as an equal-style variable, which should be specified as v_name, where name is the variable name. In this case, the variable is evaluated at the beginning of a run to determine the next timestep at which a restart file will be written out. On that timestep, the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for equal-style variables, as examples of useful functions to use in this context. Other similar math functions could easily be added as options for equal-style variables.

For example, the following commands will write restart files every step from 1100 to 1200, and could be useful for debugging a simulation where something goes wrong at step 1163:

```
variable        s equal stride(1100,1200,1)
restart         v_s tmp.restart
```

See the read_restart command for information about what is stored in a restart file.

Restart files can be read by a read_restart command to restart a simulation from a particular state. Because the file is binary (to enable exact restarts), it may not be readable on another machine. In this case, the restart2data program in the tools directory can be used to convert a restart file to an ASCII data file. Both the read_restart command and restart2data tool can read in a restart file that was written with the "%" character so that multiple files were created.

Restrictions: none

Related commands:

write_restart, read_restart

Default:

restart 0
run command

Syntax:

run N keyword values ...

- $N = \# \text{ of timesteps}$
- zero or more keyword/value pairs may be appended
- keyword = upto or start or stop or pre or post or every

`upto` value = none
`start` value = N1
  N1 = timestep at which 1st run started
`stop` value = N2
  N2 = timestep at which last run will end
`pre` value = no or yes
`post` value = no or yes
`every` values = M c1 c2 ...
  M = break the run into M-timestep segments and invoke one or more commands between each segment
  c1,c2,...,cN = one or more LAMMPS commands, each enclosed in quotes
  c1 = NULL means no command will be invoked

Examples:

run 10000
run 1000000 upto
run 100 start 0 stop 1000
run 1000 pre no post yes
run 1000000 start 0 stop 1000000 every 1000 "print 'Protein Rg = $r'"
run 100000 every 1000 NULL

Description:

Run or continue dynamics for a specified number of timesteps.

When the run style is respa, N refers to outer loop (largest) timesteps.

A value of $N = 0$ is acceptable; only the thermodynamics of the system are computed and printed without taking a timestep.

The `upto` keyword means to perform a run starting at the current timestep up to the specified timestep. E.g. if the current timestep is 10,000 and "run 100000 upto" is used, then an additional 90,000 timesteps will be run. This can be useful for very long runs on a machine that allocates chunks of time and terminate your job when time is exceeded. If you need to restart your script multiple times (reading in the last restart file), you can keep restarting your script with the same run command until the simulation finally completes.

The `start` or `stop` keywords can be used if multiple runs are being performed and you want a fix command that changes some value over time (e.g. temperature) to make the change across the entire set of runs and not just a single run. See the doc page for individual fixes to see which ones can be used with the `start/stop` keywords.

For example, consider this fix followed by 10 run commands:

```
fix 1 all nvt 200.0 300.0 1.0
run 1000 start 0 stop 10000
```
The NVT fix ramps the target temperature from 200.0 to 300.0 during a run. If the run commands did not have the start/stop keywords (just "run 1000"), then the temperature would ramp from 200.0 to 300.0 during the 1000 steps of each run. With the start/stop keywords, the ramping takes place over the 10000 steps of all runs together.

The pre and post keywords can be used to streamline the setup, clean-up, and associated output to the screen that happens before and after a run. This can be useful if you wish to do many short runs in succession (e.g. LAMMPS is being called as a library which is doing other computations between successive short LAMMPS runs).

By default (pre and post = yes), LAMMPS creates neighbor lists, computes forces, and imposes fix constraints before every run. And after every run it gathers and prints timings statistics. If a run is just a continuation of a previous run (i.e. no settings are changed), the initial computation is not necessary; the old neighbor list is still valid as are the forces. So if pre is specified as "no" then the initial setup is skipped, except for printing thermodynamic info. Note that if pre is set to "no" for the very 1st run LAMMPS performs, then it is overridden, since the initial setup computations must be done.

IMPORTANT NOTE: If your input script changes settings between 2 runs (e.g. adds a fix or dump or compute or changes a neighbor list parameter), then the initial setup must be performed. LAMMPS does not check for this, but it would be an error to use the pre no option in this case.

If post is specified as "no", the full timing summary is skipped; only a one-line summary timing is printed.

The every keyword provides a means of breaking a LAMMPS run into a series of shorter runs. Optionally, one or more LAMMPS commands (c1, c2, ..., cN) will be executed in between the short runs. If used, the every keyword must be the last keyword, since it has a variable number of arguments. Each of the trailing arguments is a single LAMMPS command, and each command should be enclosed in quotes, so that the entire command will be treated as a single argument. This will also prevent any variables in the command from being evaluated until it is executed multiple times during the run. Note that if a command itself needs one of its arguments quoted (e.g. the print command), then you can use a combination of single and double quotes, as in the example above or below.

The every keyword is a means to avoid listing a long series of runs and interleaving commands in your input script. For example, a print command could be invoked or a fix could be redefined, e.g. to reset a thermostat temperature. Or this could be useful for invoking a command you have added to LAMMPS that wraps some other code (e.g. as a library) to perform a computation periodically during a long LAMMPS run. See this section of the documentation for info about how to add new commands to LAMMPS. See this section of the documentation for ideas about how to couple LAMMPS to other codes.

With the every option, N total steps are simulated, in shorter runs of M steps each. After each M-length run, the specified commands are invoked. If only a single command is specified as NULL, then no command is invoked. Thus these lines:

```plaintext
variable q equal x[100]
run 6000 every 2000 "print Coord = $q"
```

are the equivalent of:

```plaintext
variable q equal x[100]
run 2000
print Coord = $q
run 2000
print Coord = $q
run 2000
```

1034
print Coord = $q

which does 3 runs of 2000 steps and prints the x-coordinate of a particular atom between runs. Note that the variable "$q" will be evaluated afresh each time the print command is executed.

Note that by using the line continuation character "&", the run every command can be spread across many lines, though it is still a single command:

run 100000 every 1000 &
  "print 'Minimum value = $a'" &
  "print 'Maximum value = $b'" &
  "print 'Temp = $c'" &
  "print 'Press = $d'"

If the pre and post options are set to "no" when used with the every keyword, then the 1st run will do the full setup and the last run will print the full timing summary, but these operations will be skipped for intermediate runs.

IMPORTANT NOTE: You might hope to specify a command that exits the run by jumping out of the loop, e.g.

variable t equal temp
run 10000 every 100 "if '$t <300.0' then 'jump SELF afterrun'"

Unfortunately this will not currently work. The run command simply executes each command one at a time each time it pauses, then continues the run. You can replace the jump command with a simple quit command and cause LAMMPS to exit during the middle of a run when the condition is met.

Restrictions:

The number of specified timesteps N must fit in a signed 32-bit integer, so you are limited to slightly more than 2 billion steps ($2^{31}$) in a single run. However, you can perform successive runs to run a simulation for any number of steps (ok, up to $2^{63}$ steps).

Related commands:

minimize, run_style, temper

Default:

The option defaults are start = the current timestep, stop = current timestep + N, pre = yes, and post = yes.
run_style command

Syntax:

run_style style args

- style = verlet or verlet/split or respa

  verlet args = none
  verlet/split args = none
  respa args = N n1 n2 ... keyword values ...
  N = # of levels of rRESPA
  n1, n2, ... = loop factor between rRESPA levels (N-1 values)
  zero or more keyword/value pairings may be appended to the loop factors
  keyword = bond or angle or dihedral or improper or
  pair or inner or middle or outer or kspace
  bond value = M
    M = which level (1-N) to compute bond forces in
  angle value = M
    M = which level (1-N) to compute angle forces in
  dihedral value = M
    M = which level (1-N) to compute dihedral forces in
  improper value = M
    M = which level (1-N) to compute improper forces in
  pair value = M
    M = which level (1-N) to compute pair forces in
  inner values = M cut1 cut2
    M = which level (1-N) to compute pair inner forces in
    cut1 = inner cutoff between pair inner and
    pair middle or outer (distance units)
    cut2 = outer cutoff between pair inner and
    pair middle or outer (distance units)
  middle values = M cut1 cut2
    M = which level (1-N) to compute pair middle forces in
    cut1 = inner cutoff between pair middle and pair outer (distance units)
    cut2 = outer cutoff between pair middle and pair outer (distance units)
  outer value = M
    M = which level (1-N) to compute pair outer forces in
  kspace value = M
    M = which level (1-N) to compute kspace forces in

Examples:

run_style verlet
run_style respa 4 2 2 2 bond 1 dihedral 2 pair 3 kspace 4
run_style respa 4 2 2 2 bond 1 dihedral 2 inner 3 5.0 6.0 outer 4 kspace 4

Description:

Choose the style of time integrator used for molecular dynamics simulations performed by LAMMPS.

The verlet style is a standard velocity-Verlet integrator.

The verlet/split style is also a velocity-Verlet integrator, but it splits the force calculation within each timestep over 2 partitions of processors. See Section_start 6 for an explanation of the -partition command-line switch.
Specifically, this style performs all computation except the kspace_style portion of the force field on the 1st partition. This include the pair style, bond style, neighbor list building, fixes including time integration, and output. The kspace_style portion of the calculation is performed on the 2nd partition.

This is most useful for the PPPM kspace_style when its performance on a large number of processors degrades due to the cost of communication in its 3d FFTs. In this scenario, splitting your P total processors into 2 subsets of processors, P1 in the 1st partition and P2 in the 2nd partition, can enable your simulation to run faster. This is because the long-range forces in PPPM can be calculated at the same time as pair-wise and bonded forces are being calculated, and the FFTs can actually speed up when running on fewer processors.

To use this style, you must define 2 partitions where P1 is a multiple of P2. Typically having P1 be 3x larger than P2 is a good choice. The 3d processor layouts in each partition must overlay in the following sense. If P1 is a Px1 by Py1 by Pz1 grid, and P2 = Px2 by Py2 by Pz2, then Px1 must be an integer multiple of Px2, and similarly for Py1 a multiple of Py2, and Pz1 a multiple of Pz2.

Typically the best way to do this is to let the 1st partition choose its own optimal layout, then require the 2nd partition's layout to match the integer multiple constraint. See the processors command with its part keyword for a way to control this, e.g.

```
processors * * * part 1 2 multiple
```

You can also use the partition command to explicitly specify the processor layout on each partition. E.g. for 2 partitions of 60 and 15 processors each:

```
partition yes 1 processors 3 4 5
partition yes 2 processors 3 1 5
```

When you run in 2-partition mode with the verlet/split style, the thermodynamic data for the entire simulation will be output to the log and screen file of the 1st partition, which are log.lammps.0 and screen.0 by default; see the "-plog and -pscreen command-line switches"Section_start.html#start_7 to change this. The log and screen file for the 2nd partition will not contain thermodynamic output beyone the 1st timestep of the run.

See Section_accelerate of the manual for performance details of the speed-up offered by the verlet/split style. One important performance consideration is the assignemnt of logical processors in the 2 partitions to the physical cores of a parallel machine. The processors command has options to support this, and strategies are discussed in Section_accelerate of the manual.

The respa style implements the rRESPA multi-timescale integrator (Tuckerman) with N hierarchical levels, where level 1 is the innermost loop (shortest timestep) and level N is the outermost loop (largest timestep). The loop factor arguments specify what the looping factor is between levels. N1 specifies the number of iterations of level 1 for a single iteration of level 2, N2 is the iterations of level 2 per iteration of level 3, etc. N-1 looping parameters must be specified.

The timestep command sets the timestep for the outermost rRESPA level. Thus if the example command above for a 4-level rRESPA had an outer timestep of 4.0 fmsec, the inner timestep would be 8x smaller or 0.5 fmsec. All other LAMMPS commands that specify number of timesteps (e.g. neigh_modify parameters, dump every N timesteps, etc) refer to the outermost timesteps.

The rRESPA keywords enable you to specify at what level of the hierarchy various forces will be computed. If not specified, the defaults are that bond forces are computed at level 1 (innermost loop), angle forces are computed where bond forces are, dihedral forces are computed where angle forces are, improper forces are computed where dihedral forces are, pair forces are computed at the outermost level, and kspace forces are computed where pair forces are. The inner, middle, outer forces have no defaults.
The *inner* and *middle* keywords take additional arguments for cutoffs that are used by the pairwise force computations. If the 2 cutoffs for *inner* are 5.0 and 6.0, this means that all pairs up to 6.0 apart are computed by the inner force. Those between 5.0 and 6.0 have their force go ramped to 0.0 so the overlap with the next regime (middle or outer) is smooth. The next regime (middle or outer) will compute forces for all pairs from 5.0 outward, with those from 5.0 to 6.0 having their value ramped in an inverse manner.

Only some pair potentials support the use of the *inner* and *middle* and *outer* keywords. If not, only the *pair* keyword can be used with that pair style, meaning all pairwise forces are computed at the same rRESPA level. See the doc pages for individual pair styles for details.

When using rRESPA (or for any MD simulation) care must be taken to choose a timestep size(s) that insures the Hamiltonian for the chosen ensemble is conserved. For the constant NVE ensemble, total energy must be conserved. Unfortunately, it is difficult to know *a priori* how well energy will be conserved, and a fairly long test simulation (~10 ps) is usually necessary in order to verify that no long-term drift in energy occurs with the trial set of parameters.

With that caveat, a few rules-of-thumb may be useful in selecting *respa* settings. The following applies mostly to biomolecular simulations using the CHARMM or a similar all-atom force field, but the concepts are adaptable to other problems. Without SHAKE, bonds involving hydrogen atoms exhibit high-frequency vibrations and require a timestep on the order of 0.5 fmsec in order to conserve energy. The relatively inexpensive force computations for the bonds, angles, impropers, and dihedrals can be computed on this innermost 0.5 fmsec step. The outermost timestep cannot be greater than 4.0 fmsec without risking energy drift. Smooth switching of forces between the levels of the rRESPA hierarchy is also necessary to avoid drift, and a 1-2 angstrom "healing distance" (the distance between the outer and inner cutoffs) works reasonably well. We thus recommend the following settings for use of the *respa* style without SHAKE in biomolecular simulations:

```plaintext
timestep  4.0
run_style respa 4 2 2 inner 2 4.5 6.0 middle 3 8.0 10.0 outer 4
```

With these settings, users can expect good energy conservation and roughly a 2.5 fold speedup over the *verlet* style with a 0.5 fmsec timestep.

If SHAKE is used with the *respa* style, time reversibility is lost, but substantially longer time steps can be achieved. For biomolecular simulations using the CHARMM or similar all-atom force field, bonds involving hydrogen atoms exhibit high frequency vibrations and require a time step on the order of 0.5 fmsec in order to conserve energy. These high frequency modes also limit the outer time step sizes since the modes are coupled. It is therefore desirable to use SHAKE with respa in order to freeze out these high frequency motions and increase the size of the time steps in the respa hierarchy. The following settings can be used for biomolecular simulations with SHAKE and rRESPA:

```plaintext
fix             2 all shake 0.000001 500 0 m 1.0 a 1
timestep        4.0
run_style       respa 2 2 inner 1 4.0 5.0 outer 2
```

With these settings, users can expect good energy conservation and roughly a 1.5 fold speedup over the *verlet* style with SHAKE and a 2.0 fmsec timestep.

For non-biomolecular simulations, the *respa* style can be advantageous if there is a clear separation of time scales - fast and slow modes in the simulation. Even a LJ system can benefit from rRESPA if the interactions are divided by the inner, middle and outer keywords. A 2-fold or more speedup can be obtained while maintaining good energy conservation. In real units, for a pure LJ fluid at liquid density, with a sigma of 3.0 angstroms, and epsilon of 0.1 Kcal/mol, the following settings seem to work well:

```plaintext
fstep  36.0
```
Restrictions:

The *verlet/split* style can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

Whenever using rRESPA, the user should experiment with trade-offs in speed and accuracy for their system, and verify that they are conserving energy to adequate precision.

Related commands:

timestep, run

Default:

```
run_style verlet
```

set command

Syntax:

set style ID keyword values ...

- **style** = atom or type or mol or group or region
- **ID** = atom ID range or type range or mol ID range or group ID or region ID
- one or more keyword/value pairs may be appended
- **keyword** = type or type/fraction or mol or x or y or z or charge or dipole or dipole/random or quat or quat/random or diameter or shape or length or tri or theta or angmom or mass or density or volume or image or bond or angle or dihedral or improper or meso_e or meso_cv or meso_rho

```
type value = atom type
  type/fraction values = type fraction seed
  type = new atom type
  fraction = fraction of selected atoms to set to new atom type
  seed = random # seed (positive integer)

mol value = molecule ID
  x,y,z value = atom coordinate (distance units)
  charge value = atomic charge (charge units)

  dipole values = x y z
  dipole/random value = seed Dlen
  seed = random # seed (positive integer) for dipole moment orientations
  Dlen = magnitude of dipole moment (dipole units)

quat values = a b c theta
  a,b,c = unit vector to rotate particle around via right-hand rule
  theta = rotation angle (degrees)

quat/random value = seed
  seed = random # seed (positive integer) for quaternion orientations

  diameter value = diameter of spherical particle (distance units)
  shape value = Sx Sy Sz
    Sx,Sy,Sz = 3 diameters of ellipsoid (distance units)

length value = len
  len = length of line segment (distance units)

tri value = side
  side = side length of equilateral triangle (distance units)

theta value = angle (degrees)
  angle = orientation of line segment with respect to x-axis

angmom values = Lx Ly Lz
  Lx,Ly,Lz = components of angular momentum vector (distance-mass-velocity units)

mass value = per-atom mass (mass units)

density value = particle density for sphere or ellipsoid (mass/distance^3 or mass/distance^2 or mass/distance units)
  volume value = particle volume for Peridynamic particle (distance^3 units)

image nx ny nz
  nx,ny,nz = which periodic image of the simulation box the atom is in

bond value = bond type for all bonds between selected atoms
  angle value = angle type for all angles between selected atoms

improper value = dihedral type for all dihedrals between selected atoms

meso_e value = energy of SPH particles (need units)

meso_cv value = heat capacity of SPH particles (need units)

meso_rho value = density of SPH particles (need units)
```

Examples:

set group solvent type 2
set group solvent type/fraction 2 0.5 12393
set group edge bond 4
set region half charge 0.5
set type 3 charge 0.5
set type 1*3 charge 0.5
set atom 100*200 x 0.5 y 1.0
set atom 1492 type 3

Description:

Set one or more properties of one or more atoms. Since atom properties are initially assigned by the read_data, read_restart or create_atoms commands, this command changes those assignments. This can be useful for overriding the default values assigned by the create_atoms command (e.g. charge = 0.0). It can be useful for altering pairwise and molecular force interactions, since force-field coefficients are defined in terms of types. It can be used to change the labeling of atoms by atom type or molecule ID when they are output in dump files. It can be useful for debugging purposes; i.e. positioning an atom at a precise location to compute subsequent forces or energy.

The style atom selects all the atoms in a range of atom IDs. The style type selects all the atoms in a range of types. The style mol selects all the atoms in a range of molecule IDs.

In each of the range cases, a single value can be specified, or a wildcard asterisk can be used to specify a range of values. This takes the form "*n" or "#n" or "n*" or "m*n". For example, for the style type, if N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that the lowest value for the wildcard is 1, not 0, so you cannot not use this form to select atoms with molecule ID = 0, for example.

The style group selects all the atoms in the specified group. The style region selects all the atoms in the specified geometric region. See the group and region commands for details of how to specify a group or region.

Keyword type sets the atom type for all selected atoms. The specified value must be from 1 to ntypes, where ntypes was set by the create_box command or the atom types field in the header of the data file read by the read_data command.

Keyword type/fraction sets the atom type for a fraction of the selected atoms. The actual number of atoms changed is not guaranteed to be exactly the requested fraction, but should be statistically close. Random numbers are used in such a way that a particular atom is changed or not changed, regardless of how many processors are being used.

Keyword mol sets the molecule ID for all selected atoms. The atom style being used must support the use of molecule IDs.

Keywords x, y, z, and charge set the coordinates or charge of all selected atoms. For charge, the atom style being used must support the use of atomic charge.

Keyword dipole uses the specified x,y,z values as components of a vector to set as the orientation of the dipole moment vectors of the selected atoms. The magnitude of the dipole moment is set by the length of this orientation vector.

Keyword dipole/random randomizes the orientation of the dipole moment vectors of the selected atoms and sets the magnitude of each to the specified Dlen value. For 2d systems, the z component of the orientation is set to 0.0. Random numbers are used in such a way that the orientation of a particular atom is the same, regardless of how
many processors are being used.

Keyword *quat* uses the specified values to create a quaternion (4-vector) that represents the orientation of the selected atoms. The particles must be ellipsoids as defined by the *atom_style ellipsoid* command or triangles as defined by the *atom_style tri* command. Note that particles defined by *atom_style ellipsoid* have 3 shape parameters. The 3 values must be non-zero for each particle set by this command. They are used to specify the aspect ratios of an ellipsoidal particle, which is oriented by default with its x-axis along the simulation box's x-axis, and similarly for y and z. If this body is rotated (via the right-hand rule) by an angle theta around a unit rotation vector (a,b,c), then the quaternion that represents its new orientation is given by (cos(theta/2), a*sin(theta/2), b*sin(theta/2), c*sin(theta/2)). The theta and a,b,c values are the arguments to the *quat* keyword. LAMMPS normalizes the quaternion in case (a,b,c) was not specified as a unit vector. For 2d systems, the a,b,c values are ignored, since a rotation vector of (0,0,1) is the only valid choice.

Keyword *quat/random* randomizes the orientation of the quaternion of the selected atoms. The particles must be ellipsoids as defined by the *atom_style ellipsoid* command or triangles as defined by the *atom_style tri* command. Random numbers are used in such a way that the orientation of a particular atom is the same, regardless of how many processors are being used. For 2d systems, only orientations in the xy plane are generated. As with keyword *quat*, for ellipsoidal particles, the 3 shape values must be non-zero for each particle set by this command.

Keyword *diameter* sets the size of the selected atoms. The particles must be finite-size spheres as defined by the *atom_style sphere* command. The diameter of a particle can be set to 0.0, which means they will be treated as point particles. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the *read_data* command.

Keyword *shape* sets the size and shape of the selected atoms. The particles must be ellipsoids as defined by the *atom_style ellipsoid* command. The Sx, Sy, Sz settings are the 3 diameters of the ellipsoid in each direction. All 3 can be set to the same value, which means the ellipsoid is effectively a sphere. They can also all be set to 0.0 which means the particle will be treated as a point particle. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the *read_data* command.

Keyword *length* sets the length of selected atoms. The particles must be line segments as defined by the *atom_style line* command. If the specified value is non-zero the line segment is (re)set to a length = the specified value, centered around the particle position, with an orientation along the x-axis. If the specified value is 0.0, the particle will become a point particle. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the *read_data* command.

Keyword *tri* sets the size of selected atoms. The particles must be triangles as defined by the *atom_style tri* command. If the specified value is non-zero the triangle is (re)set to be an equilateral triangle in the xy plane with side length = the specified value, with a centroid at the particle position, with its base parallel to the x axis, and the y-axis running from the center of the base to the top point of the triangle. If the specified value is 0.0, the particle will become a point particle. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the *read_data* command.

Keyword *theta* sets the orientation of selected atoms. The particles must be line segments as defined by the *atom_style line* command. The specified value is used to set the orientation angle of the line segments with respect to the x axis.

Keyword *angmom* sets the angular momentum of selected atoms. The particles must be ellipsoids as defined by the *atom_style ellipsoid* command or triangles as defined by the *atom_style tri* command. The angular momentum vector of the particles is set to the 3 specified components.

Keyword *mass* sets the mass of all selected particles. The particles must have a per-atom mass attribute, as
defined by the atom_style command. See the "mass" command for how to set mass values on a per-type basis.

Keyword density also sets the mass of all selected particles, but in a different way. The particles must have a per-atom mass attribute, as defined by the atom_style command. If the atom has a radius attribute (see atom_style sphere) and its radius is non-zero, its mass is set from the density and particle volume. If the atom has a shape attribute (see atom_style ellipsoid) and its 3 shape parameters are non-zero, then its mass is set from the density and particle volume. If the atom has a length attribute (see atom_style line) and its length is non-zero, then its mass is set from the density and line segment length (the input density is assumed to be in mass/distance units). If the atom has an area attribute (see atom_style tri) and its area is non-zero, then its mass is set from the density and triangle area (the input density is assumed to be in mass/distance^2 units). If none of these cases are valid, then the mass is set to the density value directly (the input density is assumed to be in mass units).

Keyword volume sets the volume of all selected particles. Currently, only the atom_style peri command defines particles with a volume attribute. Note that this command does not adjust the particle mass.

Keyword image sets which image of the simulation box the atom is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as atoms cross periodic boundaries during the simulation. The flags can be output with atom snapshots via the dump command. If a value of NULL is specified for any of nx,ny,nz, then the current image value for that dimension is unchanged. For non-periodic dimensions only a value of 0 can be specified.

This command can be useful after a system has been equilibrated and atoms have diffused one or more box lengths in various directions. This command can then reset the image values for atoms so that they are effectively inside the simulation box, e.g if a diffusion coefficient is about to be measured via the compute msd command. Care should be taken not to reset the image flags of two atoms in a bond to the same value if the bond straddles a periodic boundary (rather they should be different by +/- 1). This will not affect the dynamics of a simulation, but may mess up analysis of the trajectories if a LAMMPS diagnostic or your own analysis relies on the image flags to unwrap a molecule which straddles the periodic box.

Keywords bond, angle, dihedral, and improper, set the bond type (angle type, etc) of all bonds (angles, etc) of selected atoms to the specified value from 1 to nbondtypes (nangletypes, etc). All atoms in a particular bond (angle, etc) must be selected atoms in order for the change to be made. The value of nbondtype (nangletypes, etc) was set by the bond types (angle types, etc) field in the header of the data file read by the read_data command.

Keywords meso_e, meso_cv, and meso_rho set the energy, heat capacity, and density of smoothed particle hydrodynamics (SPH) particles. See this PDF guide to using SPH in LAMMPS.

Restrictions:

You cannot set an atom attribute (e.g. mol or q or volume) if the atom_style does not have that attribute.

This command requires inter-processor communication to coordinate the setting of bond types (angle types, etc). This means that your system must be ready to perform a simulation before using one of these keywords (force fields set, atom mass set, etc). This is not necessary for other keywords.

Using the region style with the bond (angle, etc) keywords can give unpredictable results if there are bonds (angles, etc) that straddle periodic boundaries. This is because the region may only extend up to the boundary and partner atoms in the bond (angle, etc) may have coordinates outside the simulation box if they are ghost atoms.

Related commands:
create_box, create_atoms, read_data

Default: none
**shell command**

**Syntax:**

```
shell cmd args
```

- `cmd = cd` or `mkdir` or `mv` or `rm` or `rmdir` or arbitrary command

  - `cd` arg = `dir`
    - `dir = directory to change to`
  - `mkdir` args = `dir1 dir2 ...`
    - `dir1, dir2 = one or more directories to create`
  - `mv` args = `old new`
    - `old = old filename`
    - `new = new filename`
  - `rm` args = `file1 file2 ...`
    - `file1, file2 = one or more filenames to delete`
  - `rmdir` args = `dir1 dir2 ...`
    - `dir1, dir2 = one or more directories to delete`

  anything else is passed as a command to the shell for direct execution

**Examples:**

```
shell cd sub1
shell cd ..
shell mkdir tmp1 tmp2 tmp3
shell rmdir tmp1
shell mv log.lammps hold/log.1
shell rm TMP/file1 TMP/file2
shell my_setup file1 10 file2
shell my_post_process 100 dump.out
```

**Description:**

Execute a shell command. A few simple file-based shell commands are supported directly, in Unix-style syntax. Any command not listed above is passed as-is to the C-library `system()` call, which invokes the command in a shell.

This is means to invoke other commands from your input script. For example, you can move files around in preparation for the next section of the input script. Or you can run a program that pre-processes data for input into LAMMPS. Or you can run a program that post-processes LAMMPS output data.

With the exception of `cd`, all commands, including ones invoked via a `system()` call, are executed by only a single processor, so that files/directories are not being manipulated by multiple processors.

The `cd` cmd executes the Unix "cd" command to change the working directory. All subsequent LAMMPS commands that read/write files will use the new directory. All processors execute this command.

The `mkdir` cmd executes the Unix "mkdir" command to create one or more directories.

The `mv` cmd executes the Unix "mv" command to rename a file and/or move it to a new directory.

The `rm` cmd executes the Unix "rm" command to remove one or more files.
The *rmdir* cmd executes the Unix "rmdir" command to remove one or more directories. A directory must be empty to be successfully removed.

Any other cmd is passed as-is to the shell along with its arguments as one string, invoked by the C-library system() call. For example, these lines in your input script:

```
variable n equal 10
variable foo string file2
shell my_setup file1 $n ${foo}
```

would be the same as invoking

```
% my_setup file1 10 file2
```

from a command-line prompt. The executable program "my_setup" is run with 3 arguments: file1 10 file2.

**Restrictions:**

LAMMPS does not detect errors or print warnings when any of these commands execute. E.g. if the specified directory does not exist, executing the *cd* command will silently do nothing.

**Related commands:** none

**Default:** none
special_bonds command

Syntax:

special_bonds keyword values ...

- one or more keyword/value pairs may be appended
- keyword = amber or charmm or dreiding or fene or lj/coul or lj or coul or angle or dihedral or extra

amber values = none
charmm values = none
dreiding values = none
fene values = none
lj/coul values = w1,w2,w3
   w1,w2,w3 = weights (0.0 to 1.0) on pairwise Lennard-Jones and Coulombic interactions
lj values = w1,w2,w3
   w1,w2,w3 = weights (0.0 to 1.0) on pairwise Lennard-Jones interactions
coul values = w1,w2,w3
   w1,w2,w3 = weights (0.0 to 1.0) on pairwise Coulombic interactions
angle value = yes or no
dihedral value = yes or no
extra value = N
   N = number of extra 1-2,1-3,1-4 interactions to save space for

Examples:

special_bonds amber
special_bonds charmm
special_bonds fene dihedral no
special_bonds lj/coul 0.0 0.0 0.5 angle yes dihedral yes
special_bonds lj 0.0 0.0 0.5 coul 0.0 0.0 0.0 dihedral yes
special_bonds lj/coul 0 1 1 extra 2

Description:

Set weighting coefficients for pairwise energy and force contributions between pairs of atoms that are also permanently bonded to each other, either directly or via one or two intermediate bonds. These weighting factors are used by nearly all pair styles in LAMMPS that compute simple pairwise interactions. Permanent bonds between atoms are specified by defining the bond topology in the data file read by the read_data command. Typically a bond_style command is also used to define a bond potential. The rationale for using these weighting factors is that the interaction between a pair of bonded atoms is all (or mostly) specified by the bond, angle, dihedral potentials, and thus the non-bonded Lennard-Jones or Coulombic interaction between the pair of atoms should be excluded (or reduced by a weighting factor).

IMPORTANT NOTE: These weighting factors are NOT used by pair styles that compute many-body interactions, since the "bonds" that result from such interactions are not permanent, but are created and broken dynamically as atom conformations change. Examples of pair styles in this category are EAM, MEAM, Stillinger-Weber, Tersoff, COMB, AIREBO, and ReaxFF. In fact, it generally makes no sense to define permanent bonds between atoms that interact via these potentials, though such bonds may exist elsewhere in your system, e.g. when using the pair_style hybrid command. Thus LAMMPS ignores special_bonds settings when manybody potentials are calculated.

The Coulomb factors are applied to any Coulomb (charge interaction) term that the potential calculates. The LJ factors are applied to the remaining terms that the potential calculates, whether they represent LJ interactions or
not. The weighting factors are a scaling pre-factor on the energy and force between the pair of atoms. A value of 1.0 means include the full interaction; a value of 0.0 means exclude it completely.

The 1st of the 3 coefficients (LJ or Coulombic) is the weighting factor on 1-2 atom pairs, which are pairs of atoms directly bonded to each other. The 2nd coefficient is the weighting factor on 1-3 atom pairs which are those separated by 2 bonds (e.g. the two H atoms in a water molecule). The 3rd coefficient is the weighting factor on 1-4 atom pairs which are those separated by 3 bonds (e.g. the 1st and 4th atoms in a dihedral interaction). Thus if the 1-2 coefficient is set to 0.0, then the pairwise interaction is effectively turned off for all pairs of atoms bonded to each other. If it is set to 1.0, then that interaction will be at full strength.

IMPORTANT NOTE: For purposes of computing weighted pairwise interactions, 1-3 and 1-4 interactions are not defined from the list of angles or dihedrals used by the simulation. Rather, they are inferred topologically from the set of bonds specified when the simulation is defined from a data or restart file (see read_data or read_restart commands). Thus the set of 1-2,1-3,1-4 interactions that the weights apply to is the same whether angle and dihedral potentials are computed or not, and remains the same even if bonds are constrained, or turned off, or removed during a simulation.

The two exceptions to this rule are (a) if the angle or dihedral keywords are set to yes (see below), or (b) if the delete_bonds command is used with the special option that recomputes the 1-2,1-3,1-4 topologies after bonds are deleted; see the delete_bonds command for more details.

The amber keyword sets the 3 coefficients to 0.0, 0.0, 0.5 for LJ interactions and to 0.0, 0.0, 0.8333 for Coulombic interactions, which is the default for a commonly used version of the AMBER force field, where the last value is really 5/6. See (Cornell) for a description of the AMBER force field.

The charmm keyword sets the 3 coefficients to 0.0, 0.0, 0.0 for both LJ and Coulombic interactions, which is the default for a commonly used version of the CHARMM force field. Note that in pair styles lj/charmm/coul/charmm and lj/charmm/coul/long the 1-4 coefficients are defined explicitly, and these pairwise contributions are computed as part of the charmm dihedral style - see the pair_coeff and dihedral_style commands for more information. See (MacKerell) for a description of the CHARMM force field.

The dreiding keyword sets the 3 coefficients to 0.0, 0.0, 1.0 for both LJ and Coulombic interactions, which is the default for the Dreiding force field, as discussed in (Mayo).

The fene keyword sets the 3 coefficients to 0.0, 1.0, 1.0 for both LJ and Coulombic interactions, which is consistent with a coarse-grained polymer model with FENE bonds. See (Kremer) for a description of FENE bonds.

The lj/coul, lj, and coul keywords allow the 3 coefficients to be set explicitly. The lj/coul keyword sets both the LJ and Coulombic coefficients to the same 3 values. The lj and coul keywords only set either the LJ or Coulombic coefficients. Use both of them if you wish to set the LJ coefficients to different values than the Coulombic coefficients.

The angle keyword allows the 1-3 weighting factor to be ignored for individual atom pairs if they are not listed as the first and last atoms in any angle defined in the simulation or as 1,3 or 2,4 atoms in any dihedral defined in the simulation. For example, imagine the 1-3 weighting factor is set to 0.5 and you have a linear molecule with 4 atoms and bonds as follows: 1-2-3-4. If your data file defines 1-2-3 as an angle, but does not define 2-3-4 as an angle or 1-2-3-4 as a dihedral, then the pairwise interaction between atoms 1 and 3 will always be weighted by 0.5, but different force fields use different rules for weighting the pairwise interaction between atoms 2 and 4. If the angle keyword is specified as yes, then the pairwise interaction between atoms 2 and 4 will be unaffected (full weighting of 1.0). If the angle keyword is specified as no which is the default, then the 2,4 interaction will also be weighted by 0.5.
The *dihedral* keyword allows the 1-4 weighting factor to be ignored for individual atom pairs if they are not listed as the first and last atoms in any dihedral defined in the simulation. For example, imagine the 1-4 weighting factor is set to 0.5 and you have a linear molecule with 5 atoms and bonds as follows: 1-2-3-4-5. If your data file defines 1-2-3-4 as a dihedral, but does not define 2-3-4-5 as a dihedral, then the pairwise interaction between atoms 1 and 4 will always be weighted by 0.5, but different force fields use different rules for weighting the pairwise interaction between atoms 2 and 5. If the *dihedral* keyword is specified as *yes*, then the pairwise interaction between atoms 2 and 5 will be unaffected (full weighting of 1.0). If the *dihedral* keyword is specified as *no* which is the default, then the 2,5 interaction will also be weighted by 0.5.

The *extra* keyword is used when additional bonds will be created during a simulation run, e.g. by the *fix bond/create* command. A list of 1-2,1-3,1-4 neighbors for each atom is calculated and stored by LAMMPS. If new bonds are created, the list needs to grow. Using the *extra* keyword leaves empty space in the list for N additional bonds to be added. If you do not do this, you may get an error when bonds are added.

**Restrictions:** none

**Related commands:**

*delete_bonds, fix bond/create*

**Default:**

All 3 Lennard-Jones and 3 Coulombic weighting coefficients = 0.0, angle = no, dihedral = no, and extra = 0.


suffix command

Syntax:

suffix style

- style = off or on or opt or omp or gpu or cuda

Examples:

suffix off
suffix on
suffix gpu

Description:

This command allows you to use variants of various styles if they exist. In that respect it operates the same as the -suffix command-line switch. It also has options to turn off/on any suffix setting made via the command line.

The specified style can be opt, omp, gpu, or cuda. These refer to optional packages that LAMMPS can be built with, as described in this section of the manual. The "opt" style corresponds to the OPT package, the "omp" style to the USER-OMP package, the "gpu" style to the GPU package, and the "cuda" style to the USER-CUDA package.

These are the variants these packages provide:

- OPT = a handful of pair styles, cache-optimized for faster CPU performance
- USER-OMP = a collection of pair, bond, angle, dihedral, improper, kspace, compute, and fix styles with support for OpenMP multi-threading
- GPU = a handful of pair styles and the PPPM kspace_style, optimized to run on one or more GPUs or multicore CPU/GPU nodes
- USER-CUDA = a collection of atom, pair, fix, compute, and intergrate styles, optimized to run on one or more NVIDIA GPUs

As an example, all of the packages provide a pair_style lj/cut variant, with style names lj/cut/opt, lj/cut/omp, lj/cut/gpu, or lj/cut/cuda. A variant styles can be specified explicitly in your input script, e.g. pair_style lj/cut/gpu. If the suffix command is used with the appropriate style, you do not need to modify your input script. The specified suffix (opt,omp,gpu,cuda) is automatically appended whenever your input script command creates a new atom, pair, bond, angle, dihedral, improper, kspace, fix, compute, or run style. If the variant version does not exist, the standard version is created.

If the specified style is off, then any previously specified suffix is temporarily disabled, whether it was specified by a command-line switch or a previous suffix command. If the specified style is on, a disabled suffix is turned back on. The use of these 2 commands lets your input script use a standard LAMMPS style (i.e. a non-accelerated variant), which can be useful for testing or benchmarking purposes. Of course this is also possible by not using any suffix commands, and explicitly appending or not appending the suffix to the relevant commands in your input script.

Restrictions: none

Related commands:
Command-line switch -suffix

Default: none
**tad command**

**Syntax:**

```
tad N t_event T_lo T_hi delta tmax compute-ID keyword value ... 
```

- **N** = # of timesteps to run (not including dephasing/quenching)
- **t_event** = timestep interval between event checks
- **T_lo** = temperature at which event times are desired
- **T_hi** = temperature at which MD simulation is performed
- **delta** = desired confidence level for stopping criterion
- **tmax** = reciprocal of lowest expected preexponential factor (time units)
- **compute-ID** = ID of the compute used for event detection
- **zero or more keyword/value pairs may be appended**
- **keyword** = *min* or *neb* or *min_style* or *neb_style* or *neb_log*

**Examples:**

```
tad 2000 50 1800 2300 0.01 0.01 event
```

**Description:**

Run a temperature accelerated dynamics (TAD) simulation. This method requires two or more partitions to perform NEB transition state searches.

TAD is described in [this paper](#) by Art Voter. It is a method that uses accelerated dynamics at an elevated temperature to generate results at a specified lower temperature. A good overview of accelerated dynamics methods for such systems is given in [this review paper](#) from the same group. In general, these methods assume that the long-time dynamics is dominated by infrequent events i.e. the system is is confined to low energy basins for long periods, punctuated by brief, randomly-occurring transitions to adjacent basins. TAD is suitable for infrequent-event systems, where in addition, the transition kinetics are well-approximated by harmonic transition state theory (hTST). In hTST, the temperature dependence of transition rates follows the Arrhenius relation. As a consequence a set of event times generated in a high-temperature simulation can be mapped to a set of much...
longer estimated times in the low-temperature system. However, because this mapping involves the energy barrier of the transition event, which is different for each event, the first event at the high temperature may not be the earliest event at the low temperature. TAD handles this by first generating a set of possible events from the current basin. After each event, the simulation is reflected backwards into the current basin. This is repeated until the stopping criterion is satisfied, at which point the event with the earliest low-temperature occurrence time is selected. The stopping criterion is that the confidence measure be greater than 1-\(\delta\). The confidence measure is the probability that no earlier low-temperature event will occur at some later time in the high-temperature simulation. hTST provides a lower bound for this probability, based on the user-specified minimum pre-exponential factor (reciprocal of \(t_{max}\)).

In order to estimate the energy barrier for each event, the TAD method invokes the NEB method. Each NEB replica runs on a partition of processors. The current NEB implementation in LAMMPS restricts you to having exactly one processor per replica. For more information, see the documentation for the neb command. In the current LAMMPS implementation of TAD, all the non-NEB TAD operations are performed on the first partition, while the other partitions remain idle. See Section_howto 5 of the manual for further discussion of multi-replica simulations.

A TAD run has several stages, which are repeated each time an event is performed. The logic for a TAD run is as follows:

\[
\text{while (time remains)}:
\quad \text{while (time < tstop)}:
\quad \quad \text{until (event occurs)}:
\quad \quad \quad \text{run dynamics for t_event steps}
\quad \quad \quad \text{quench}
\quad \quad \quad \text{run neb calculation using all replicas}
\quad \quad \quad \text{compute tlo from energy barrier}
\quad \quad \quad \text{update earliest event}
\quad \quad \quad \text{update tstop}
\quad \quad \quad \text{reflect back into current basin}
\quad \quad \quad \text{execute earliest event}
\]

Before this outer loop begins, the initial potential energy basin is identified by quenching (an energy minimization, see below) the initial state and storing the resulting coordinates for reference.

Inside the inner loop, dynamics is run continuously according to whatever integrator has been specified by the user, stopping every \(t_{event}\) steps to check if a transition event has occurred. This check is performed by quenching the system and comparing the resulting atom coordinates to the coordinates from the previous basin.

A quench is an energy minimization and is performed by whichever algorithm has been defined by the \text{min} \hspace{1em} \text{and} \hspace{1em} \text{min_style} \hspace{1em} keywords or their default values. Note that typically, you do not need to perform a highly-converged minimization to detect a transition event.

The event check is performed by a compute with the specified compute-ID. Currently there is only one compute that works with the TAD command, which is the compute event/displace command. Other event-checking computes may be added. Compute event/displace checks whether any atom in the compute group has moved further than a specified threshold distance. If so, an "event" has occurred.

The neb calculation is similar to that invoked by the neb command, except that the final state is generated internally, instead of being read in from a file. The TAD implementation provides default values for the NEB settings, which can be overridden using the neb and neb_style keywords.

A key aspect of the TAD method is setting the stopping criterion appropriately. If this criterion is too conservative, then many events must be generated before one is finally executed. Conversely, if this criterion is
too aggressive, high-entropy high-barrier events will be over-sampled, while low-entropy low-barrier events will be under-sampled. If the lowest pre-exponential factor is known fairly accurately, then it can be used to estimate $t_{max}$, and the value of $delta$ can be set to the desired confidence level e.g. $delta = 0.05$ corresponds to 95% confidence. However, for systems where the dynamics are not well characterized (the most common case), it will be necessary to experiment with the values of $delta$ and $t_{max}$ to get a good trade-off between accuracy and performance.

A second key aspect is the choice of $t_{hi}$. A larger value greatly increases the rate at which new events are generated. However, too large a value introduces errors due to anharmonicity (not accounted for within hTST). Once again, for any given system, experimentation is necessary to determine the best value of $t_{hi}$.

Five kinds of output can be generated during a TAD run: event statistics, NEB statistics, thermodynamic output by each replica, dump files, and restart files.

Event statistics are printed to the screen and master log.lammps file each time an event is executed. The quantities are the timestep, CPU time, global event number $N$, local event number $M$, event status, energy barrier, time margin, $t_{lo}$ and $delt_{lo}$. The timestep is the usual LAMMPS timestep, which corresponds to the high-temperature time at which the event was detected, in units of timestep. The CPU time is the total processor time since the start of the TAD run. The global event number $N$ is a counter that increments with each executed event. The local event number $M$ is a counter that resets to zero upon entering each new basin. The event status is $E$ when an event is executed, and is $D$ for an event that is detected, while $DF$ is for a detected event that is also the earliest (first) event at the low temperature.

The time margin is the ratio of the high temperature time in the current basin to the stopping time. This last number can be used to judge whether the stopping time is too short or too long (see above).

$t_{lo}$ is the low-temperature event time when the current basin was entered, in units of timestep. $delt_{lo}$ is the time of each detected event, measured relative to $t_{lo}$. $delt_{lo}$ is equal to the high-temperature time since entering the current basin, scaled by an exponential factor that depends on the hi/lo temperature ratio and the energy barrier for that event.

On lines for executed events, with status $E$, the global event number is incremented by one, the local event number and time margin are reset to zero, while the global event number, energy barrier, and $delt_{lo}$ match the last event with status $DF$ in the immediately preceding block of detected events. The low-temperature event time $t_{lo}$ is incremented by $delt_{lo}$.

The NEB statistics are written to the file specified by the $neb\_log$ keyword. If the keyword value is "none", then no NEB statistics are printed out. The statistics are written every $Nevery$ timesteps. See the $neb$ command for a full description of the NEB statistics. When invoked from TAD, NEB statistics are never printed to the screen.

Because the NEB calculation must run on multiple partitions, LAMMPS produces additional screen and log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For the TAD command, these contain the thermodynamic output of each NEB replica. In addition, the log file for the first partition, log.lammps.0, will contain thermodynamic output from short runs and minimizations corresponding to the dynamics and quench operations, as well as a line for each new detected event, as described above.

After the TAD command completes, timing statistics for the TAD run are printed in each replica's log file, giving a breakdown of how much CPU time was spent in each stage (NEB, dynamics, quenching, etc).

Any dump files defined in the input script will be written to during a TAD run at timesteps when an event is executed. This means the the requested dump frequency in the $dump$ command is ignored. There will be one dump file (per dump command) created for all partitions. The atom coordinates of the dump snapshot are those of
the minimum energy configuration resulting from quenching following the executed event. The timesteps written into the dump files correspond to the timestep at which the event occurred and NOT the clock. A dump snapshot corresponding to the initial minimum state used for event detection is written to the dump file at the beginning of each TAD run.

If the `restart` command is used, a single restart file for all the partitions is generated, which allows a TAD run to be continued by a new input script in the usual manner. The restart file is generated after an event is executed. The restart file contains a snapshot of the system in the new quenched state, including the event number and the low-temperature time. The restart frequency specified in the `restart` command is interpreted differently when performing a TAD run. It does not mean the timestep interval between restart files. Instead it means an event interval for executed events. Thus a frequency of 1 means write a restart file every time an event is executed. A frequency of 10 means write a restart file every 10th executed event. When an input script reads a restart file from a previous TAD run, the new script can be run on a different number of replicas or processors.

Note that within a single state, the dynamics will typically temporarily continue beyond the event that is ultimately chosen, until the stopping criterion is satisfied. When the event is eventually executed, the timestep counter is reset to the value when the event was detected. Similarly, after each quench and NEB minimization, the timestep counter is reset to the value at the start of the minimization. This means that the timesteps listed in the replica log files do not always increase monotonically. However, the timestep values printed to the master log file, dump files, and restart files are always monotonically increasing.

**Restrictions:**

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

\[ N \text{ setting must be integer multiple of } t_{\text{event}}. \]

Runs restarted from restart files written during a TAD run will only produce identical results if the user-specified integrator supports exact restarts. So `fix nvt` will produce an exact restart, but `fix langevin` will not.

This command cannot be used when any fixes are defined that keep track of elapsed time to perform time-dependent operations. Examples include the "ave" fixes such as `fix ave/spatial`. Also `fix dt/reset` and `fix deposit`.

**Related commands:**

`compute event/displace`, `min_modify`, `min_style`, `run_style`, `minimize`, `temper`, `neb`, `prd`

**Default:**

The option defaults are `min = 0.1 0.1 40 50`, `neb = 0.01 100 100 10`, `min_style = cg`, `neb_style = quickmin`, and `neb_log = "none"`


temper command

Syntax:

```
temper N M temp fix-ID seed1 seed2 index
```

- **N** = total # of timesteps to run
- **M** = attempt a tempering swap every this many steps
- **temp** = initial temperature for this ensemble
- **fix-ID** = ID of the fix that will control temperature during the run
- **seed1** = random # seed used to decide on adjacent temperature to partner with
- **seed2** = random # seed for Boltzmann factor in Metropolis swap
- **index** = which temperature (0 to N-1) I am simulating (optional)

Examples:

```
temper 100000 100 $t tempfix 0 58728
temper 40000 100 $t tempfix 0 32285 $w
```

Description:

Run a parallel tempering or replica exchange simulation using multiple replicas (ensembles) of a system. Two or more replicas must be used.

Each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the -partition command-line switch; see Section_start 6 of the manual. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g. you can run a 10-replica simulation on one or two processors. You will simply not get the performance speed-up you would see with one or more physical processors per replica. See this section of the manual for further discussion.

Each replica’s temperature is controlled at a different value by a fix with fix-ID that controls temperature. Possible fix styles are nvt, temp/berendsen, langevin and temp/rescale. The desired temperature is specified by temp, which is typically a variable previously set in the input script, so that each partition is assigned a different temperature. See the variable command for more details. For example:

```
variable t world 300.0 310.0 320.0 330.0
fix myfix all nvt $t $t 100.0
temper 100000 100 $t myfix 3847 58382
```

would define 4 temperatures, and assign one of them to the thermostat used by each replica, and to the temper command.

As the tempering simulation runs for N timesteps, a temperature swap between adjacent ensembles will be attempted every M timesteps. If seed1 is 0, then the swap attempts will alternate between odd and even pairings. If seed1 is non-zero then it is used as a seed in a random number generator to randomly choose an odd or even pairing each time. Each attempted swap of temperatures is either accepted or rejected based on a Boltzmann-weighted Metropolis criterion which uses seed2 in the random number generator.

As a tempering run proceeds, multiple log files and screen output files are created, one per replica. By default these files are named log.lammps.M and screen.M where M is the replica number from 0 to N-1, with N = # of replicas. See the section on command-line switches for info on how to change these names.
The main screen and log file (log.lammps) will list information about which temperature is assigned to each replica at each thermodynamic output timestep. E.g. for a simulation with 16 replicas:

```
Running on 16 partitions of processors
Step T0 T1 T2 T3 T4 T5 T6 T7 T8 T9 T10 T11 T12 T13 T14 T15
 0  0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
500 1 0 3 2 5 4 6 7 8 9 10 11 12 13 14 15
1000 2 0 4 1 5 3 6 7 8 9 10 11 12 14 13 15
1500 2 1 4 0 5 3 6 7 9 8 10 11 12 14 13 15
2000 2 1 3 0 6 4 5 7 10 8 9 11 12 14 13 15
2500 2 1 3 0 6 4 5 7 11 8 9 10 12 14 13 15
...```

The column headings T0 to TN-1 mean which temperature is currently assigned to the replica 0 to N-1. Thus the columns represent replicas and the value in each column is its temperature (also numbered 0 to N-1). For example, a 0 in the 4th column (column T3, step 2500) means that the 4th replica is assigned temperature 0, i.e. the lowest temperature. You can verify this time sequence of temperature assignments for the Nth replica by comparing the Nth column of screen output to the thermodynamic data in the corresponding log.lammps.N or screen.N files as time proceeds.

The last argument index in the temper command is optional and is used when restarting a tempering run from a set of restart files (one for each replica) which had previously swapped to new temperatures. The index value (from 0 to N-1, where N is the # of replicas) identifies which temperature the replica was simulating on the timestep the restart files were written. Obviously, this argument must be a variable so that each partition has the correct value. Set the variable to the N values listed in the log file for the previous run for the replica temperatures at that timestep. For example if the log file listed the following for a simulation with 5 replicas:

```
500000 2 4 0 1 3```

then a setting of

```
variable w world 2 4 0 1 3```

would be used to restart the run with a tempering command like the example above with $w as the last argument.

**Restrictions:**

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

**Related commands:**

variable, prd, neb

**Default:** none
thermo command

Syntax:

```
thermo N
```

- N = output thermodynamics every N timesteps
- N can be a variable (see below)

Examples:

```
thermo 100
```

Description:

Compute and print thermodynamic info (e.g. temperature, energy, pressure) on timesteps that are a multiple of N and at the beginning and end of a simulation. A value of 0 will only print thermodynamics at the beginning and end.

The content and format of what is printed is controlled by the thermo_style and thermo_modify commands.

Instead of a numeric value, N can be specified as an equal-style variable, which should be specified as v_name, where name is the variable name. In this case, the variable is evaluated at the beginning of a run to determine the next timestep at which thermodynamic info will be written out. On that timestep, the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for equal-style variables, as examples of useful functions to use in this context. Other similar math functions could easily be added as options for equal-style variables.

For example, the following commands will output thermodynamic info at timesteps 0,10,20,30,100,200,300,1000,2000,etc:

```
variable        s equal logfreq(10,3,10)
thermo          v_s
```

Restrictions: none

Related commands:

thermo_style, thermo_modify

Default:

```
thermo 0
```
thermo_modify command

Syntax:

thermo_modify keyword value ...

- one or more keyword/value pairs may be listed

  keyword = lost or norm or flush or line or format or temp
  or press

  value = error or warn or ignore norm value = yes or no flush value = yes or no
  line value = one or multi format values = int string or float string or M
  string M = integer from 1 to N, where N = # of
  quantities being printed

  string = C-style format string

  temp value = compute ID that calculates a
  temperature

  press value = compute ID that calculates a pressure

Examples:

thermo_modify lost ignore flush yes
thermo_modify temp myTemp format 3 %15.8g
thermo_modify line multi format float %g

Description:

Set options for how thermodynamic information is computed and printed by LAMMPS.

IMPORTANT NOTE: These options apply to the currently defined thermo style. When you specify a
thermo_style command, all thermodynamic settings are restored to their default values, including those previously
reset by a thermo_modify command. Thus if your input script specifies a thermo_style command, you should use
the thermo_modify command after it.

The lost keyword determines whether LAMMPS checks for lost atoms each time it computes thermodynamics
and what it does if atoms are lost. An atom can be "lost" if it moves across a non-periodic simulation box
boundary or if it moves more than a box length outside the simulation domain (or more than a processor
sub-domain length) before reneighboring occurs. The latter case is typically due to bad dynamics, e.g. too large a
timestep or huge forces and velocities. If the value is ignore, LAMMPS does not check for lost atoms. If the value
is error or warn, LAMMPS checks and either issues an error or warning. The code will exit with an error and
continue with a warning. A warning will only be issued once, the first time an atom is lost. This can be a useful
debugging option.

The norm keyword determines whether various thermodynamic output values are normalized by the number of
atoms or not, depending on whether it is set to yes or no. Different unit styles have different defaults for this
setting (see below). Even if norm is set to yes, a value is only normalized if it is an "extensive" quantity, meaning
that it scales with the number of atoms in the system. For the thermo keywords described by the doc page for the
thermo_style command, all energy-related keywords are extensive, such as pe or ebond or enthalpy. Other
keywords such as temp or press are "intensive" meaning their value is independent (in a statistical sense) of the
number of atoms in the system and thus are never normalized. For thermodynamic output values extracted from
fixes and computes in a thermo_style custom command, the doc page for the individual fix or compute lists
whether the value is "extensive" or "intensive" and thus whether it is normalized. Thermodynamic output values
calculated by a variable formula are assumed to be "intensive" and thus are never normalized. You can always
include a divide by the number of atoms in the variable formula if this is not the case.

The flush keyword invokes a flush operation after thermodynamic info is written to the log file. This insures the
output in that file is current (no buffering by the OS), even if LAMMPS halts before the simulation completes.
The *line* keyword determines whether thermodynamics will be printed as a series of numeric values on one line or in a multi-line format with 3 quantities with text strings per line and a dashed-line header containing the timestep and CPU time. This modify option overrides the *one* and *multi* thermo_style settings.

The *format* keyword sets the numeric format of individual printed quantities. The *int* and *float* keywords set the format for all integer or floating-point quantities printed. The setting with a numeric value M (e.g., format 5 %10.4g) sets the format of the Mth value printed in each output line, e.g., the 5th column of output in this case. If the format for a specific column has been set, it will take precedence over the *int* or *float* setting.

IMPORTANT NOTE: The thermo output values *step* and *atoms* are stored internally as 8-byte signed integers, rather than the usual 4-byte signed integers. When specifying the "format int" keyword you can use a "%d"-style format identifier in the format string and LAMMPS will convert this to the corresponding "%lu" form when it is applied to those keywords. However, when specifying the "format M string" keyword for *step* and *natoms*, you should specify a string appropriate for an 8-byte signed integer, e.g., one with "%ld".

The *temp* keyword is used to determine how thermodynamic temperature is calculated, which is used by all thermo quantities that require a temperature ("temp", "press", "ke", "etotal", "enthalpy", "pxx", etc). The specified compute ID must have been previously defined by the user via the compute command and it must be a style of compute that calculates a temperature. As described in the thermo_style command, thermo output uses a default compute for temperature with ID = thermo_temp. This option allows the user to override the default.

The *press* keyword is used to determine how thermodynamic pressure is calculated, which is used by all thermo quantities that require a pressure ("press", "enthalpy", "pxx", etc). The specified compute ID must have been previously defined by the user via the compute command and it must be a style of compute that calculates a pressure. As described in the thermo_style command, thermo output uses a default compute for pressure with ID = thermo_press. This option allows the user to override the default.

IMPORTANT NOTE: If both the *temp* and *press* keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a pressure compute defines its own temperature compute as an argument when it is specified. The *temp* keyword will override this (for the pressure compute being used by thermodynamics), but only if the *temp* keyword comes after the *press* keyword. If the *temp* keyword comes before the *press* keyword, then the new pressure compute specified by the *press* keyword will be unaffected by the *temp* setting.

**Restrictions:** none

**Related commands:**

thermo, thermo_style

**Default:**

The option defaults are lost = error, norm = yes for unit style of lj, norm = no for unit style of real and metal, flush = no, and temp/press = compute IDs defined by thermo_style.

The defaults for the line and format options depend on the thermo style. For styles "one" and "custom", the line and format defaults are "one", "%8d", and "%12.8g". For style "multi", the line and format defaults are "multi", "%8d", and "%14.4f".
thermo_style command

Syntax:

thermo_style style args

- style = one or multi or custom
- args = list of arguments for a particular style

one args = none
multi args = none
custom args = list of attributes

possible attributes = step, elapsed, elaplong, dt, cpu, tpcpu, spcpu,
atoms, temp, press, pe, ke, etotal, enthalpy,
evdlw, ecoul, epair, ebond, eangle, edihed, eimp,
emol, elong, etail,
vol, lx, ly, lz, xlo, xhi, ylo, yhi, zlo, zhi,
xy, xz, yz, xlat, ylat, zlat,
pxx, pyy, pzz, pxy, pxz, pyz,
fmax, fnorm,
cella, cellb, cellc, cellalpha, cellbeta, cellgamma,
c_ID, c_ID[I], c_ID[I][J],
f_ID, f_ID[I], f_ID[I][J],
v_name

step = timestep
elapsed = timesteps since start of this run
elaplong = timesteps since start of initial run in a series of runs
dt = timestep size
cpu = elapsed CPU time in seconds
tpcpu = time per CPU second
spcpu = timesteps per CPU second
atoms = # of atoms
temp = temperature
press = pressure
pe = total potential energy
ke = kinetic energy
etotal = total energy (pe + ke)
enthalpy = enthalpy (etotal + press*vol)
evdlw = VanderWaal pairwise energy
ecoul = Coulombic pairwise energy
epair = pairwise energy (evdlw + ecoul + elong + etail)
ebond = bond energy
eangle = angle energy
edihed = dihedral energy
eimp = improper energy
emol = molecular energy (ebond + eangle + edihed + eimp)
elong = long-range kspace energy
etail = VanderWaal energy long-range tail correction
vol = volume
lx,ly,lz = box lengths in x,y,z
xlo,xhi,ylo,yhi,zlo,zhi = box boundaries
xy,xz,yz = box tilt for triclinic (non-orthogonal) simulation boxes
xlat,ylat,zlat = lattice spacings as calculated by lattice command
pxx,pyy,pzz,pxy,pxz,pyz = 6 components of pressure tensor
fmax = max component of force on any atom in any dimension
fnorm = length of force vector for all atoms
cella,cellb,cellc = periodic cell lattice constants a,b,c
cellalpha, cellbeta, cellgamma = periodic cell angles alpha,beta,gamma
c_ID = global scalar value calculated by a compute with ID
c_ID[I] = Ith component of global vector calculated by a compute with ID
c_ID[I][J] = I,J component of global array calculated by a compute with ID
f_ID = global scalar value calculated by a fix with ID
f_ID[I] = Ith component of global vector calculated by a fix with ID
f_ID[I][J] = I,J component of global array calculated by a fix with ID
v_name = scalar value calculated by an equal-style variable with name

Examples:

thermo_style multi
thermo_style custom step temp pe etotal press vol
thermo_style custom step temp etotal c_myTemp v_abc

Description:

Set the style and content for printing thermodynamic data to the screen and log file.

Style one prints a one-line summary of thermodynamic info that is the equivalent of "thermo_style custom step temp epair emol etotal press". The line contains only numeric values.

Style multi prints a multiple-line listing of thermodynamic info that is the equivalent of "thermo_style custom etotal ke temp pe ebond eangle edihed eimp evdwl ecoul elong press". The listing contains numeric values and a string ID for each quantity.

Style custom is the most general setting and allows you to specify which of the keywords listed above you want printed on each thermodynamic timestep. Note that the keywords c_ID, f_ID, v_name are references to computes, fixes, and equal-style variables that have been defined elsewhere in the input script or can even be new styles which users have added to LAMMPS (see the Section_modify section of the documentation). Thus the custom style provides a flexible means of outputting essentially any desired quantity as a simulation proceeds.

All styles except custom have vol appended to their list of outputs if the simulation box volume changes during the simulation.

The values printed by the various keywords are instantaneous values, calculated on the current timestep. Time-averaged quantities, which include values from previous timesteps, can be output by using the f_ID keyword and accessing a fix that does time-averaging such as the fix ave/time command.

Options invoked by the thermo_modify command can be used to set the one- or multi-line format of the print-out, the normalization of thermodynamic output (total values versus per-atom values for extensive quantities (ones which scale with the number of atoms in the system), and the numeric precision of each printed value.

IMPORTANT NOTE: When you use a "thermo_style" command, all thermodynamic settings are restored to their default values, including those previously set by a thermo_modify command. Thus if your input script specifies a thermo_style command, you should use the thermo_modify command after it.

Several of the thermodynamic quantities require a temperature to be computed: "temp", "press", "ke", "etotal", "enthalpy", "pxx", etc. By default this is done by using a temperature compute which is created when LAMMPS starts up, as if this command had been issued:

compute thermo_temp all temp

See the compute temp command for details. Note that the ID of this compute is thermo_temp and the group is all. You can change the attributes of this temperature (e.g. its degrees-of-freedom) via the compute_modify command. Alternatively, you can directly assign a new compute (that calculates temperature) which you have defined, to be used for calculating any thermodynamic quantity that requires a temperature. This is done via the
Several of the thermodynamic quantities require a pressure to be computed: "press", "enthalpy", "pxx", etc. By default this is done by using a pressure compute which is created when LAMMPS starts up, as if this command had been issued:

compute thermo_press all pressure thermo_temp

See the compute pressure command for details. Note that the ID of this compute is thermo_press and the group is all. You can change the attributes of this pressure via the compute_modify command. Alternatively, you can directly assign a new compute (that calculates pressure) which you have defined, to be used for calculating any thermodynamic quantity that requires a pressure. This is done via the thermo_modify command.

Several of the thermodynamic quantities require a potential energy to be computed: "pe", "etotal", "ebond", etc. This is done by using a pe compute which is created when LAMMPS starts up, as if this command had been issued:

compute thermo_pe all pe

See the compute pe command for details. Note that the ID of this compute is thermo_pe and the group is all. You can change the attributes of this potential energy via the compute_modify command.

The kinetic energy of the system $ke$ is inferred from the temperature of the system with 1/2 Kb T of energy for each degree of freedom. Thus, using different compute commands for calculating temperature, via the thermo_modify temp command, may yield different kinetic energies, since different computes that calculate temperature can subtract out different non-thermal components of velocity and/or include different degrees of freedom (translational, rotational, etc).

The potential energy of the system $pe$ will include contributions from fixes if the fix_modify thermo option is set for a fix that calculates such a contribution. For example, the fix wall/lj93 fix calculates the energy of atoms interacting with the wall. See the doc pages for "individual fixes" to see which ones contribute.

A long-range tail correction $etail$ for the VanderWaal pairwise energy will be non-zero only if the pair_modify tail option is turned on. The $etail$ contribution is included in $evdwl$, $pe$, and $etotal$, and the corresponding tail correction to the pressure is included in $press$ and $pxx$, $pyy$, etc.

The step, elapsed, and elaplong keywords refer to timestep count. Step is the current timestep, or iteration count when a minimization is being performed. Elapsed is the number of timesteps elapsed since the beginning of this run. Elaplong is the number of timesteps elapsed since the beginning of an initial run in a series of runs. See the start and stop keywords for the run for info on how to invoke a series of runs that keep track of an initial starting time. If these keywords are not used, then elapsed and elaplong are the same value.

The cpu keyword is elapsed CPU seconds since the beginning of this run. The tpcpu and spcpu keywords are measures of how fast your simulation is currently running. The tpcpu keyword is simulation time per CPU second, where simulation time is in time units. E.g. for metal units, the tpcpu value would be picoseconds per CPU second. The spcpu keyword is the number of timesteps per CPU second. Both quantities are on-the-fly metrics, measured relative to the last time they were invoked. Thus if you are printing out thermodynamic output every 100 timesteps, the two keywords will continually output the time and timestep rate for the last 100 steps.

The tpcpu keyword does not attempt to track any changes in timestep size, e.g. due to using the fix dt/reset command.

The fmax and fnorm keywords are useful for monitoring the progress of an energy minimization. The fmax
keyword calculates the maximum force in any dimension on any atom in the system, or the infinity-norm of the force vector for the system. The \textit{fnorm} keyword calculates the 2-norm or length of the force vector.

The keywords \textit{cella, cellb, celtc, cellalpha, cellbeta, cellgamma}, correspond to the usual crystallographic quantities that define the periodic unit cell of a crystal. See this section of the doc pages for a geometric description of triclinic periodic cells, including a precise definition of these quantities in terms of the internal LAMMPS cell dimensions $l_x, l_y, l_z, yz, xz, xy$.

The \textit{c\_ID} and \textit{c\_ID[I]} and \textit{c\_ID[I][J]} keywords allow global values calculated by a compute to be output. As discussed on the compute doc page, computes can calculate global, per-atom, or local values. Only global values can be referenced by this command. However, per-atom compute values can be referenced in a \textit{variable} and the variable referenced by thermo\_style custom, as discussed below.

The ID in the keyword should be replaced by the actual ID of a compute that has been defined elsewhere in the input script. See the compute command for details. If the compute calculates a global scalar, vector, or array, then the keyword formats with 0, 1, or 2 brackets will reference a scalar value from the compute.

Note that some computes calculate "intensive" global quantities like temperature; others calculate "extensive" global quantities like kinetic energy that are summed over all atoms in the compute group. Intensive quantities are printed directly without normalization by thermo\_style custom. Extensive quantities may be normalized by the total number of atoms in the simulation (NOT the number of atoms in the compute group) when output, depending on the thermo\_modify norm option being used.

The \textit{f\_ID} and \textit{f\_ID[I]} and \textit{f\_ID[I][J]} keywords allow global values calculated by a fix to be output. As discussed on the fix doc page, fixes can calculate global, per-atom, or local values. Only global values can be referenced by this command. However, per-atom fix values can be referenced in a \textit{variable} and the variable referenced by thermo\_style custom, as discussed below.

The ID in the keyword should be replaced by the actual ID of a fix that has been defined elsewhere in the input script. See the fix command for details. If the fix calculates a global scalar, vector, or array, then the keyword formats with 0, 1, or 2 brackets will reference a scalar value from the fix.

Note that some fixes calculate "intensive" global quantities like timestep size; others calculate "extensive" global quantities like energy that are summed over all atoms in the fix group. Intensive quantities are printed directly without normalization by thermo\_style custom. Extensive quantities may be normalized by the total number of atoms in the simulation (NOT the number of atoms in the fix group) when output, depending on the thermo\_modify norm option being used.

The \textit{v\_name} keyword allow the current value of a variable to be output. The name in the keyword should be replaced by the variable name that has been defined elsewhere in the input script. Only equal-style variables can be referenced. See the variable command for details. Variables of style equal can reference per-atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when evaluated, so this is a very general means of creating thermodynamic output.

See Section\_modify for information on how to add new compute and fix styles to LAMMPS to calculate quantities that can then be referenced with these keywords to generate thermodynamic output.

\textbf{Restrictions:}

This command must come after the simulation box is defined by a \texttt{read\_data, read\_restart, or create\_box} command.
Related commands:

thermo, thermo_modify, fix_modify, compute temp, compute pressure

Default:

thermo_style one
timestep command

Syntax:

timestep dt

- dt = timestep size (time units)

Examples:

timestep 2.0

timestep 0.003

Description:

Set the timestep size for subsequent molecular dynamics simulations. See the units command for a discussion of time units. The default value for the timestep also depends on the choice of units for the simulation; see the default values below.

When the run style is respa, dt is the timestep for the outer loop (largest) timestep.

Restrictions: none

Related commands:

fix dt/reset, run, run_style respa, units

Default:

timestep = 0.005 tau for units = lj

timestep = 1.0 fmsec for units = real

timestep = 0.001 psec for units = metal

timestep = 1.0e-8 sec (10 nsec) for units = si or cgs
uncompute command

Syntax:

uncompute compute-ID

• compute-ID = ID of a previously defined compute

Examples:

uncompute 2
uncompute lower-boundary

Description:

Delete a compute that was previously defined with a compute command. This also wipes out any additional changes made to the compute via the compute_modify command.

Restrictions: none

Related commands:

compute

Default: none
undump command

Syntax:

undump dump-ID

- dump-ID = ID of previously defined dump

Examples:

undump mine
undump 2

Description:

Turn off a previously defined dump so that it is no longer active. This closes the file associated with the dump.

Restrictions: none

Related commands:

dump

Default: none
unfix command

Syntax:

unfix fix-ID

- fix-ID = ID of a previously defined fix

Examples:

unfix 2
unfix lower-boundary

Description:

Delete a fix that was previously defined with a fix command. This also wipes out any additional changes made to the fix via the fix_modify command.

Restrictions: none

Related commands:

fix

Default: none
units command

Syntax:

units style

  • style = lj or real or metal or si or cgs or electron

Examples:

units metal
units lj

Description:

This command sets the style of units used for a simulation. It determines the units of all quantities specified in the input script and data file, as well as quantities output to the screen, log file, and dump files. Typically, this command is used at the very beginning of an input script.

For all units except lj, LAMMPS uses physical constants from www.physics.nist.gov. For the definition of Kcal in real units, LAMMPS uses the thermochemical calorie = 4.184 J.

For style lj, all quantities are unitless. Without loss of generality, LAMMPS sets the fundamental quantities mass, sigma, epsilon, and the Boltzmann constant = 1. The masses, distances, energies you specify are multiples of these fundamental values. The formulas relating the reduced or unitless quantity (with an asterisk) to the same quantity with units is also given. Thus you can use the mass & sigma & epsilon values for a specific material and convert the results from a unitless LJ simulation into physical quantities.

  • mass = mass or m
  • distance = sigma, where x* = x / sigma
  • time = tau, where tau = t* = t (epsilon / m / sigma^2)^1/2
  • energy = epsilon, where E* = E / epsilon
  • velocity = sigma/tau, where v* = v tau / sigma
  • force = epsilon/sigma, where f* = f sigma / epsilon
  • torque = epsilon, where t* = t / epsilon
  • temperature = reduced LJ temperature, where T* = T Kb / epsilon
  • pressure = reduced LJ pressure, where P* = P sigma^3 / epsilon
  • dynamic viscosity = reduced LJ viscosity, where eta* = eta sigma^3 / epsilon / tau
  • charge = reduced LJ charge, where q* = q / (4 pi perm0 sigma epsilon)^(1/2)
  • dipole = reduced LJ dipole, moment where *mu = mu / (4 pi perm0 sigma^3 epsilon)^(1/2)
  • electric field = force/charge, where E* = E (4 pi perm0 sigma epsilon)^(1/2) sigma / epsilon
  • density = mass/volume, where rho* = rho sigma^dim

Note that for LJ units, the default mode of thermodynamic output via the thermo_style command is to normalize energies by the number of atoms, i.e. energy/atom. This can be changed via the thermo_modify norm command.

For style real, these are the units:

  • mass = grams/mole
  • distance = Angstroms
• time = femtoseconds
• energy = Kcal/mole
• velocity = Angstroms/femtosecond
• force = Kcal/mole-Angstrom
• torque = Kcal/mole
• temperature = degrees K
• pressure = atmospheres
• dynamic viscosity = Poise
• charge = multiple of electron charge (+1.0 is a proton)
• dipole = charge*Angstroms
• electric field = volts/Angstrom
• density = gram/cm^dim

For style metal, these are the units:

• mass = grams/mole
• distance = Angstroms
• time = picoseconds
• energy = eV
• velocity = Angstroms/picosecond
• force = eV/Angstrom
• torque = eV
• temperature = degrees K
• pressure = bars
• dynamic viscosity = Poise
• charge = multiple of electron charge (+1.0 is a proton)
• dipole = charge*Angstroms
• electric field = volts/Angstrom
• density = gram/cm^dim

For style si, these are the units:

• mass = kilograms
• distance = meters
• time = seconds
• energy = Joules
• velocity = meters/second
• force = Newtons
• torque = Newton-meters
• temperature = degrees K
• pressure = Pascals
• dynamic viscosity = Pascal*second
• charge = Coulombs
• dipole = Coulombs*meters
• electric field = volts/meter
• density = kilograms/meter^dim

For style cgs, these are the units:

• mass = grams
• distance = centimeters
• time = seconds
- energy = ergs
- velocity = centimeters/second
- force = dynes
- torque = dyne-centimeters
- temperature = degrees K
- pressure = dyne/cm^2 or barye = 1.0e-6 bars
- dynamic viscosity = Poise
- charge = statcoulombs or esu
- dipole = statcoul-cm = 10^18 debye
- electric field = statvolt/cm or dyne/esu
- density = grams/cm^dim

For style *electron*, these are the units:

- mass = atomic mass units
- distance = Bohr
- time = femtoseconds
- energy = Hartrees
- velocity = Bohr/atomic time units [1.03275e-15 seconds]
- force = Hartrees*Bohr
- temperature = degrees K
- pressure = Pascals
- charge = multiple of electron charge (+1.0 is a proton)
- dipole moment = Debye
- electric field = volts/cm

The units command also sets the timestep size and neighbor skin distance to default values for each style:

- For style *lj* these are dt = 0.005 tau and skin = 0.3 sigma.
- For style *real* these are dt = 1.0 fmsec and skin = 2.0 Angstroms.
- For style *metal* these are dt = 0.001 psec and skin = 2.0 Angstroms.
- For style *si* these are dt = 1.0e-8 sec and skin = 0.001 meters.
- For style *cgs* these are dt = 1.0e-8 sec and skin = 0.1 cm.
- For style *electron* these are dt = 0.001 fmsec and skin = 2.0 Bohr.

**Restrictions:**

This command cannot be used after the simulation box is defined by a *read_data* or *create_box* command.

**Related commands:** none

**Default:**

`units lj`
variable command

Syntax:

variable name style args ...

- name = name of variable to define
- style = delete or index or loop or world or universe or uloop or string or equal or atom

delete = no args

index args = one or more strings

loop args = N
- N = integer size of loop, loop from 1 to N inclusive
- pad = all values will be same length, e.g. 001, 002, ..., 100

loop args = N1 N2
- N1, N2 = loop from N1 to N2 inclusive
- pad = all values will be same length, e.g. 050, 051, ..., 100

world args = one string for each partition of processors

universe args = one or more strings

uloop args = N
- N = integer size of loop
- pad = all values will be same length, e.g. 001, 002, ..., 100

string args = one string

equal or atom args = one formula containing numbers, thermo keywords, math operations, group functions

constants = PI

thermo keywords = vol, ke, press, etc from thermo_style

math operators = (), -x, x+y, x-y, x*y, x/y, x^y, x=x, x!=y, x>=y, x&&y, x||y, !x

math functions = sqrt(x), exp(x), ln(x), log(x), sin(x), cos(x), tan(x), asin(x), acos(x), atan(x), atan2(y,x), random(x,y,z), normal(x,y,z), ceil(x), floor(x), round(x)

group functions = count(group), mass(group), charge(group), xcm(group,dim), vcm(group,dim), fcm(group,dim), bound(group,xmin), gyration(group), angmom(group,dim), torque(group,dim), inertia(group,dim), omega(group,dim)

region functions = count(group,region), mass(group,region), charge(group,region), xcm(group,dim,region), vcm(group,dim,region), fcm(group,dim,region), bound(group,xmin,region), gyration(group,region), angmom(group,dim,region), torque(group,dim,region), inertia(group,dim,region), omega(group,dim,region)

special functions = sum(x), min(x), max(x), ave(x), trap(x), gmask(x), rmask(x), grmask(x), atom value = mass[i], type[i], x[i], y[i], z[i], vx[i], vy[i], vz[i], fx[i], fy[i], fz[i]

atom vector = mass, type, x, y, z, vx, vy, vz, fx, fy, fz

compute references = c_ID, c_ID[i], c_ID[i][j]

fix references = f_ID, f_ID[i], f_ID[i][j]

variable references = v_name, v_name[i]

Examples:

variable x index run1 run2 run3 run4 run5 run6 run7 run8
variable LoopVar loop $n
variable beta equal temp/3.0
variable b1 equal x[234]+0.5*vol
variable b1 equal "x[234] + 0.5*vol"
variable b equal xcm(mol1,x)/2.0
variable b equal c_myTemp
variable b atom x*y/vol
variable foo string myfile
variable temp world 300.0 310.0 320.0 ${Tfinal}
variable x universe 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
variable x uloop 15 pad
variable x delete

Description:

This command assigns one or more strings to a variable name for evaluation later in the input script or during a simulation.

Variables can be used in several ways in LAMMPS. A variable can be referenced elsewhere in an input script to become part of a new input command. For variable styles that store multiple strings, the next command can be used to increment which string is assigned to the variable. Variables of style equal store a formula which when evaluated produces a single numeric value which can be output either directly (see the print, fix print, and run every commands) or as part of thermodynamic output (see the thermo_style command), or used as input to an averaging fix (see the fix ave/time command). Variables of style atom store a formula which when evaluated produces one numeric value per atom which can be output to a dump file (see the dump custom command) or used as input to an averaging fix (see the fix ave/spatial and fix ave/atom commands).

In the discussion that follows, the "name" of the variable is the arbitrary string that is the 1st argument in the variable command. This name can only contain alphanumeric characters and underscores. The "string" is one or more of the subsequent arguments. The "string" can be simple text as in the 1st example above, it can contain other variables as in the 2nd example, or it can be a formula as in the 3rd example. The "value" is the numeric quantity resulting from evaluation of the string. Note that the same string can generate different values when it is evaluated at different times during a simulation.

IMPORTANT NOTE: When the input script line that defines a variable of style equal or atom that contain a formula is encountered, the formula is NOT immediately evaluated and the result stored. See the discussion below about "Immediate Evaluation of Variables" if you want to do this.

IMPORTANT NOTE: When a variable command is encountered in the input script and the variable name has already been specified, the command is ignored. This means variables can NOT be re-defined in an input script (with 2 exceptions, read further). This is to allow an input script to be processed multiple times without resetting the variables; see the jump or include commands. It also means that using the command-line switch -var will override a corresponding index variable setting in the input script.

There are two exceptions to this rule. First, variables of style string and equal and atom ARE redefined each time the command is encountered. This allows these style of variables to be redefined multiple times in an input script. In a loop, this means the formula associated with an equal or atom style variable can change if it contains a substitution for another variable, e.g. $x.

Second, as described below, if a variable is iterated on to the end of its list of strings via the next command, it is removed from the list of active variables, and is thus available to be re-defined in a subsequent variable command. The delete style does the same thing.

This section of the manual explains how occurrences of a variable name in an input script line are replaced by the
variable’s string. The variable name can be referenced as $x if the name "x" is a single character, or as ${LoopVar} if the name "LoopVar" is one or more characters.

As described below, for variable styles index, loop, universe, and uloop, which string is assigned to a variable can be incremented via the next command. When there are no more strings to assign, the variable is exhausted and a flag is set that causes the next jump command encountered in the input script to be skipped. This enables the construction of simple loops in the input script that are iterated over and then exited from.

As explained above, an exhausted variable can be re-used in an input script. The delete style also removes the variable, the same as if it were exhausted, allowing it to be redefined later in the input script or when the input script is looped over. This can be useful when breaking out of a loop via the if and jump commands before the variable would become exhausted. For example,

```plaintext
label       loop
variable    a loop 5
print        "A = $a"
if           "$a > 2" then "jump in.script break"
next         a
jump         in.script loop
label        break
variable     a delete
```

For the index style, one or more strings are specified. Initially, the 1st string is assigned to the variable. Each time a next command is used with the variable name, the next string is assigned. All processors assign the same string to the variable.

Index style variables with a single string value can also be set by using the command-line switch -var; see this section for details.

The loop style is identical to the index style except that the strings are the integers from 1 to N inclusive, if only one argument N is specified. This allows generation of a long list of runs (e.g. 1000) without having to list N strings in the input script. Initially, the string "1" is assigned to the variable. Each time a next command is used with the variable name, the next string ("2", "3", etc) is assigned. All processors assign the same string to the variable. The loop style can also be specified with two arguments N1 and N2. In this case the loop runs from N1 to N2 inclusive, and the string N1 is initially assigned to the variable. N1 <= N2 and N2 >= 0 is required.

For the world style, one or more strings are specified. There must be one string for each processor partition or "world". See this section of the manual for information on running LAMMPS with multiple partitions via the "-partition" command-line switch. This variable command assigns one string to each world. All processors in the world are assigned the same string. The next command cannot be used with equal style variables, since there is only one value per world. This style of variable is useful when you wish to run different simulations on different partitions, or when performing a parallel tempering simulation (see the temper command), to assign different temperatures to different partitions.

For the universe style, one or more strings are specified. There must be at least as many strings as there are processor partitions or "worlds". See this page for information on running LAMMPS with multiple partitions via the "-partition" command-line switch. This variable command initially assigns one string to each world. When a next command is encountered using this variable, the first processor partition to encounter it, is assigned the next available string. This continues until all the variable strings are consumed. Thus, this command can be used to run 50 simulations on 8 processor partitions. The simulations will be run one after the other on whatever partition becomes available, until they are all finished. Universe style variables are incremented using the files "tmp.lammps.variable" and "tmp.lammps.variable.lock" which you will see in your directory during such a LAMMPS run.
The *uloop* style is identical to the *universe* style except that the strings are the integers from 1 to N. This allows generation of long list of runs (e.g. 1000) without having to list N strings in the input script.

For the *equal* and *atom* styles, a single string is specified which represents a formula that will be evaluated afresh each time the variable is used. If you want spaces in the string, enclose it in double quotes so the parser will treat it as a single argument. For *equal* style variables the formula computes a scalar quantity, which becomes the value of the variable whenever it is evaluated. For *atom* style variables the formula computes one quantity for each atom whenever it is evaluated.

Note that *equal* and *atom* variables can produce different values at different stages of the input script or at different times during a run. For example, if an *equal* variable is used in a fix print command, different values could be printed each timestep it was invoked. If you want a variable to be evaluated immediately, so that the result is stored by the variable instead of the string, see the section below on "Immediate Evaluation of Variables".

The next command cannot be used with *equal* or *atom* style variables, since there is only one string.

The formula for an *equal* or *atom* variable can contain a variety of quantities. The syntax for each kind of quantity is simple, but multiple quantities can be nested and combined in various ways to build up formulas of arbitrary complexity. For example, this is a valid (though strange) variable formula:

```
variable x equal "pe + c_MyTemp / vol^(1/3)"
```

Specifically, an formula can contain numbers, thermo keywords, math operators, math functions, group functions, region functions, atom values, atom vectors, compute references, fix references, and references to other variables.

<table>
<thead>
<tr>
<th>Number</th>
<th>0.2, 100, 1.0e20, -15.4, etc</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant</td>
<td>PI</td>
</tr>
<tr>
<td>Thermo keywords</td>
<td>vol, pe, ebond, etc</td>
</tr>
<tr>
<td>Math operators</td>
<td>(, -x, x+y, x-y, x*y, x/y, x^y, x==y, x!=y, xy, x&gt;=y, x&amp;&amp;y, x</td>
</tr>
<tr>
<td>Math functions</td>
<td>sqrt(x), exp(x), ln(x), log(x), sin(x), cos(x), tan(x), asin(x), acos(x), atan(x), atan2(y,x), random(x,y,z), normal(x,y,z), ceil(x), floor(x), round(x), ramp(x,y), stagger(x,y), logfreq(x,y,z), stride(x,y,z), vdisplace(x,y), swiggle(x,y,z), cwiggle(x,y,z)</td>
</tr>
<tr>
<td>Group functions</td>
<td>count(ID), mass(ID), charge(ID), xcm(ID,dim), vcm(ID,dim), fcm(ID,dim), bound(ID,dim), gyration(ID), ke(ID), angmom(ID,dim), torque(ID,dim), inertia(ID,dim), omega(ID,dim)</td>
</tr>
<tr>
<td>Region functions</td>
<td>count(ID,IDR), mass(ID,IDR), charge(ID,IDR), xcm(ID,dim,IDR), vcm(ID,dim,IDR), fcm(ID,dim,IDR), bound(ID,dim,IDR), gyration(ID,IDR), ke(ID,IDR), angmom(ID,dim,IDR), torque(ID,dim,IDR), inertia(ID,dim,IDR), omega(ID,dim,IDR)</td>
</tr>
<tr>
<td>Special functions</td>
<td>sum(x), min(x), max(x), ave(x), trap(x), gmask(x), rmask(x), grmask(x,y)</td>
</tr>
<tr>
<td>Atom values</td>
<td>mass[i], type[i], x[i], y[i], z[i], vx[i], vy[i], vz[i], fx[i], fy[i], fz[i]</td>
</tr>
<tr>
<td>Atom vectors</td>
<td>mass, type, x, y, z, vx, vy, vz, fx, fy, fz</td>
</tr>
<tr>
<td>Compute references</td>
<td>c_ID, c_ID[i], c_ID[i][j]</td>
</tr>
<tr>
<td>Fix references</td>
<td>f_ID, f_ID[i], f_ID[i][j]</td>
</tr>
<tr>
<td>Other variables</td>
<td>v_name, v_name[i]</td>
</tr>
</tbody>
</table>
Most of the formula elements produce a scalar value. A few produce a per-atom vector of values. These are the atom vectors, compute references that represent a per-atom vector, fix references that represent a per-atom vector, and variables that are atom-style variables. Math functions that operate on scalar values produce a scalar value; math function that operate on per-atom vectors do so element-by-element and produce a per-atom vector.

A formula for equal-style variables cannot use any formula element that produces a per-atom vector. A formula for an atom-style variable can use formula elements that produce either a scalar value or a per-atom vector.

Atom-style variables are evaluated by other commands that define a group on which they operate, e.g. a dump or compute or fix command. When they invoke the atom-style variable, only atoms in the group are included in the formula evaluation. The variable evaluates to 0.0 for atoms not in the group.

The thermo keywords allowed in a formula are those defined by the thermo_style custom command. Thermo keywords that require a compute to calculate their values such as "temp" or "press", use computes stored and invoked by the thermo_style command. This means that you can only use those keywords in a variable if the style you are using with the thermo_style command (and the thermo keywords associated with that style) also define and use the needed compute. Note that some thermo keywords use a compute indirectly to calculate their value (e.g. the enthalpy keyword uses temp, pe, and pressure). If a variable is evaluated directly in an input script (not during a run), then the values accessed by the thermo keyword must be current. See the discussion below about "Variable Accuracy".

Math Operators

Math operators are written in the usual way, where the "x" and "y" in the examples can themselves be arbitrarily complex formulas, as in the examples above. In this syntax, "x" and "y" can be scalar values or per-atom vectors. For example, "ke/natoms" is the division of two scalars, where "vy+vz" is the element-by-element sum of two per-atom vectors of y and z velocities.

Operators are evaluated left to right and have the usual C-style precedence: unary minus and unary logical NOT operator "!" have the highest precedence, exponentiation "^" is next; multiplication and division are next; addition and subtraction are next; the 4 relational operators """, and ">=" are next; the two remaining relational operators "==" and "!=" are next; then the logical AND operator "&&"; and finally the logical OR operator "||" has the lowest precedence. Parenthesis can be used to group one or more portions of a formula and/or enforce a different order of evaluation than what would occur with the default precedence.

The 6 relational operators return either a 1.0 or 0.0 depending on whether the relationship between x and y is TRUE or FALSE. For example the expression x

These relational and logical operators can be used as a masking or selection operation in a formula. For example, the number of atoms whose properties satisfy one or more criteria could be calculated by taking the returned per-atom vector of ones and zeroes and passing it to the compute reduce command.

Math Functions

Math functions are specified as keywords followed by one or more parenthesized arguments "x", "y", "z", each of which can themselves be arbitrarily complex formulas. In this syntax, the arguments can represent scalar values or per-atom vectors. In the latter case, the math operation is performed on each element of the vector. For example, "sqrt(natoms)" is the sqrt() of a scalar, where "sqrt(y*z)" yields a per-atom vector with each element being the sqrt() of the product of one atom's y and z coordinates.

Most of the math functions perform obvious operations. The ln() is the natural log; log() is the base 10 log.
The random(x,y,z) function takes 3 arguments: x = lo, y = hi, and z = seed. It generates a uniform random number between lo and hi. The normal(x,y,z) function also takes 3 arguments: x = mu, y = sigma, and z = seed. It generates a Gaussian variate centered on mu with variance sigma^2. In both cases the seed is used the first time the internal random number generator is invoked, to initialize it. For equal-style variables, every processor uses the same seed so that they each generate the same sequence of random numbers. For atom-style variables, a unique seed is created for each processor, based on the specified seed. This effectively generates a different random number for each atom being looped over in the atom-style variable.

IMPORTANT NOTE: Internally, there is just one random number generator for all equal-style variables and one for all atom-style variables. If you define multiple variables (of each style) which use the random() or normal() math functions, then the internal random number generators will only be initialized once, which means only one of the specified seeds will determine the sequence of generated random numbers.

The ceil(), floor(), and round() functions are those in the C math library. Ceil() is the smallest integer not less than its argument. Floor() if the largest integer not greater than its argument. Round() is the nearest integer to its argument.

The ramp(x,y) function uses the current timestep to generate a value linearly interpolated between the specified x,y values over the course of a run, according to this formula:

\[ \text{value} = x + (y-x) \times \frac{\text{timestep} - \text{startstep}}{\text{stopstep} - \text{startstep}} \]

The run begins on startstep and ends on stopstep. Startstep and stopstep can span multiple runs, using the start and stop keywords of the run command. See the run command for details of how to do this.

The stagger(x,y) function uses the current timestep to generate a new timestep. X,y > 0 and x > y are required. The generated timesteps increase in a staggered fashion, as the sequence x,x+y,2x,2x+y,3x,3x+y,etc. For any current timestep, the next timestep in the sequence is returned. Thus if stagger(1000,100) is used in a variable by the dump_modify every command, it will generate the sequence of output timesteps:

100,1000,1100,2000,2100,3000,etc

The logfreq(x,y,z) function uses the current timestep to generate a new timestep. X,y,z > 0 and y < z are required. The generated timesteps increase in a logarithmic fashion, as the sequence x,2x,3x,...y*x,z*x,2*z*x,3*z*x,...y*z*x,z*z*x,2*z*x*x,etc. For any current timestep, the next timestep in the sequence is returned. Thus if logfreq(100,4,10) is used in a variable by the dump_modify every command, it will generate the sequence of output timesteps:

100,200,300,400,1000,2000,3000,4000,10000,20000,etc

The stride(x,y,z) function uses the current timestep to generate a new timestep. X,y >= 0 and z > 0 and x <= y are required. The generated timesteps increase in increments of z, from x to y, i.e. it generates the sequence x,x+z,x+2z,...,y. If y-x is not a multiple of z, then similar to the way a for loop operates, the last value will be one that does not exceed y. For any current timestep, the next timestep in the sequence is returned. Thus if stagger(1000,2000,100) is used in a variable by the dump_modify every command, it will generate the sequence of output timesteps:

1000,1100,1200, ... ,1900,2000

The vdisplace(x,y) function takes 2 arguments: x = value0 and y = velocity, and uses the elapsed time to change the value by a linear displacement due to the applied velocity over the course of a run, according to this formula:

\[ \text{value} = \text{value0} + \text{velocity} \times (\text{timestep} - \text{startstep}) \times \text{dt} \]
where \( dt = \) the timestep size.

The run begins on startstep. Startstep can span multiple runs, using the `start` keyword of the `run` command. See the `run` command for details of how to do this. Note that the `thermo_style` keyword `elaplong = timestep-startstep`.

The `swiggle(x,y,z)` and `cwiggle(x,y,z)` functions each take 3 arguments: \( x = \) value\(_0\), \( y = \) amplitude, \( z = \) period. They use the elapsed time to oscillate the value by a \( \sin() \) or \( \cos() \) function over the course of a run, according to one of these formulas, where \( \omega = \frac{2 \pi}{\text{period}} \):

\[
\text{value} = \text{value}_0 + \text{Amplitude} \times \sin(\omega \times (\text{timestep}-\text{startstep}) \times \text{dt}) \\
\text{value} = \text{value}_0 + \text{Amplitude} \times (1 - \cos(\omega \times (\text{timestep}-\text{startstep}) \times \text{dt}))
\]

where \( dt = \) the timestep size.

The run begins on startstep. Startstep can span multiple runs, using the `start` keyword of the `run` command. See the `run` command for details of how to do this. Note that the `thermo_style` keyword `elaplong = timestep-startstep`.

---

**Group and Region Functions**

Group functions are specified as keywords followed by one or two parenthesized arguments. The first argument is the group-ID. The `dim` argument, if it exists, is \( x \) or \( y \) or \( z \). The `dir` argument, if it exists, is \( xmin \), \( xmax \), \( ymin \), \( ymax \), \( zmin \), or \( zmax \). The `dimdim` argument, if it exists, is \( xx \) or \( yy \) or \( zz \) or \( xy \) or \( yz \) or \( xz \).

The group function `count()` is the number of atoms in the group. The group functions `mass()` and `charge()` are the total mass and charge of the group. `Xcm()` and `vcm()` return components of the position and velocity of the center of mass of the group. `Fcm()` returns a component of the total force on the group of atoms. `Bound()` returns the min/max of a particular coordinate for all atoms in the group. `Gyration()` computes the radius-of-gyration of the group of atoms. See the `compute gyration` command for a definition of the formula. `Angmom()` returns components of the angular momentum of the group of atoms around its center of mass. `Torque()` returns components of the torque on the group of atoms around its center of mass, based on current forces on the atoms. `Inertia()` returns one of 6 components of the inertia tensor of the group of atoms around its center of mass. `Omega()` returns components of the angular velocity of the group of atoms around its center of mass.

Region functions are specified exactly the same way as group functions except they take an extra argument which is the region ID. The function is computed for all atoms that are in both the group and the region. If the group is "all", then the only criteria for atom inclusion is that it be in the region.

---

**Special Functions**

Special functions take specific kinds of arguments, meaning their arguments cannot be formulas themselves.

The `sum(x)`, `min(x)`, `max(x)`, `ave(x)`, and `trap(x)` functions each take 1 argument which is of the form "\( c_{\text{ID}} \)" or "\( c_{\text{ID}}[N] \)" or "\( f_{\text{ID}} \)" or "\( f_{\text{ID}}[N] \)". The first two are computes and the second two are fixes; the ID in the reference should be replaced by the ID of a compute or fix defined elsewhere in the input script. The compute or fix must produce either a global vector or array. If it produces a global vector, then the notation without "\([N]\)" should be used. If it produces a global array, then the notation with "\([N]\)" should be used, when \( N \) is an integer, to specify which column of the global array is being referenced.

These functions operate on the global vector of inputs and reduce it to a single scalar value. This is analoguous to the operation of the `compute reduce` command, which invokes the same functions on per-atom and local vectors.

The `sum()` function calculates the sum of all the vector elements. The `min()` and `max()` functions find the
minimum and maximum element respectively. The ave() function is the same as sum() except that it divides the result by the length of the vector. The trap() function is the same as sum() except the first and last elements are multiplied by a weighting factor of 1/2 when performing the sum. This effectively implements an integration via the trapezoidal rule on the global vector of data. I.e. consider a set of points, equally spaced by 1 in their x coordinate: (1,V1), (2,V2), ..., (N,VN), where the V_i are the values in the global vector of length N. The integral from 1 to N of these points is trap(). When appropriately normalized by the timestep size, this function is useful for calculating integrals of time-series data, like that generated by the fix ave/correlate command.

The gmask(x) function takes 1 argument which is a group ID. It can only be used in atom-style variables. It returns a 1 for atoms that are in the group, and a 0 for atoms that are not.

The rmask(x) function takes 1 argument which is a region ID. It can only be used in atom-style variables. It returns a 1 for atoms that are in the geometric region, and a 0 for atoms that are not.

The grmask(x,y) function takes 2 arguments. The first is a group ID, and the second is a region ID. It can only be used in atom-style variables. It returns a 1 for atoms that are in both the group and region, and a 0 for atoms that are not in both.

---

### Atom Values and Vectors

Atom values take a single integer argument I from 1 to N, where I is the an atom-ID, e.g. x[243], which means use the x coordinate of the atom with ID = 243.

Atom vectors generate one value per atom, so that a reference like "vx" means the x-component of each atom's velocity will be used when evaluating the variable. Note that other atom attributes can be used as inputs to a variable by using the compute property/atom command and then specifying a quantity from that compute.

---

### Compute References

Compute references access quantities calculated by a compute. The ID in the reference should be replaced by the ID of a compute defined elsewhere in the input script. As discussed in the doc page for the compute command, computes can produce global, per-atom, or local values. Only global and per-atom values can be used in a variable. Computes can also produce a scalar, vector, or array. An equal-style variable can only use scalar values, which means a global scalar, or an element of a global or per-atom vector or array. Atom-style variables can use the same scalar values. They can also use per-atom vector values. A vector value can be a per-atom vector itself, or a column of an per-atom array. See the doc pages for individual computes to see what kind of values they produce.

Examples of different kinds of compute references are as follows. There is no ambiguity as to what a reference means, since computes only produce global or per-atom quantities, never both.

<table>
<thead>
<tr>
<th>c_ID</th>
<th>global scalar, or per-atom vector</th>
</tr>
</thead>
<tbody>
<tr>
<td>c_ID[I]</td>
<td>Ith element of global vector, or atom I's value in per-atom vector, or Ith column from per-atom array</td>
</tr>
<tr>
<td>c_ID[I][J]</td>
<td>I,J element of global array, or atom I's Jth value in per-atom array</td>
</tr>
</tbody>
</table>

If a variable containing a compute is evaluated directly in an input script (not during a run), then the values accessed by the compute must be current. See the discussion below about "Variable Accuracy".
Fix References

Fix references access quantities calculated by a fix. The ID in the reference should be replaced by the ID of a fix defined elsewhere in the input script. As discussed in the doc page for the fix command, fixes can produce global, per-atom, or local values. Only global and per-atom values can be used in a variable. Fixes can also produce a scalar, vector, or array. An equal-style variable can only use scalar values, which means a global scalar, or an element of a global or per-atom vector or array. Atom-style variables can use the same scalar values. They can also use per-atom vector values. A vector value can be a per-atom vector itself, or a column of an per-atom array. See the doc pages for individual fixes to see what kind of values they produce.

The different kinds of fix references are exactly the same as the compute references listed in the above table, where "c_" is replaced by "f_". Again, there is no ambiguity as to what a reference means, since fixes only produce global or per-atom quantities, never both.

<table>
<thead>
<tr>
<th>f_ID</th>
<th>global scalar, or per-atom vector</th>
</tr>
</thead>
<tbody>
<tr>
<td>f_ID[I]</td>
<td>Ith element of global vector, or atom I's value in per-atom vector, or Ith column from per-atom array</td>
</tr>
<tr>
<td>f_ID[I][J]</td>
<td>I,J element of global array, or atom I's Jth value in per-atom array</td>
</tr>
</tbody>
</table>

If a variable containing a fix is evaluated directly in an input script (not during a run), then the values accessed by the fix should be current. See the discussion below about "Variable Accuracy".

Note that some fixes only generate quantities on certain timesteps. If a variable attempts to access the fix on non-allowed timesteps, an error is generated. For example, the fix ave/time command may only generate averaged quantities every 100 steps. See the doc pages for individual fix commands for details.

Variable References

Variable references access quantities calculated by other variables, which will cause those variables to be evaluated. The name in the reference should be replaced by the name of a variable defined elsewhere in the input script. As discussed on this doc page, atom-style variables generate a per-atom vector of values; all other variable styles generate a global scalar value. An equal-style variable can only use scalar values, which means another equal-style variable or an element of an atom-style variable. Atom-style variables can use the same scalar values. They can also use other atom-style variables.

Examples of different kinds of variable references are as follows. There is no ambiguity as to what a reference means, since variables produce only a global scalar or a per-atom vectors, never both.

<table>
<thead>
<tr>
<th>v_name</th>
<th>scalar, or per-atom vector</th>
</tr>
</thead>
<tbody>
<tr>
<td>v_name[I]</td>
<td>atom I's value in per-atom vector</td>
</tr>
</tbody>
</table>

IMPORTANT NOTE: If you define variables in circular manner like this:

```plaintext
variable a equal v_b
variable b equal v_a
print $a
```

then LAMMPS may run for a while when the print statement is invoked!

Immediate Evaluation of Variables:

There is a difference between referencing a variable with a leading $ sign (e.g. $x or ${abc}) versus with a leading "v_" (e.g. v_x or v_abc). The former can be used in any command, including a variable command, to force the immediate evaluation of the referenced variable and the substitution of its value into the command. The
latter is a required kind of argument to some commands (e.g. the fix ave/spatial or dump custom or thermo_style commands) if you wish it to evaluate a variable periodically during a run. It can also be used in a variable formula if you wish to reference a second variable. The second variable will be evaluated whenever the first variable is evaluated.

As an example, suppose you use this command in your input script to define the variable "v" as

\[ \text{variable } v \text{ equal } \text{vol} \]

before a run where the simulation box size changes. You might think this will assign the initial volume to the variable "v". That is not the case. Rather it assigns a formula which evaluates the volume (using the thermo_style keyword "vol") to the variable "v". If you use the variable "v" in some other command like fix ave/time then the current volume of the box will be evaluated continuously during the run.

If you want to store the initial volume of the system, you can do it this way:

\[ \text{variable } v \text{ equal } \text{vol} \]
\[ \text{variable } v0 \text{ equal } $v \]

The second command will force "v" to be evaluated (yielding the initial volume) and assign that value to the variable "v0". Thus the command

\[ \text{thermo_style custom step v}_v \ v_v0 \]

would print out both the current and initial volume periodically during the run.

Note that it is a mistake to enclose a variable formula in double quotes if it contains variables preceeded by $ signs. For example,

\[ \text{variable vratio equal } "\{vfinal}\/{v0}\" \]

This is because the quotes prevent variable substitution (see this section on parsing input script commands), and thus an error will occur when the formula for "vratio" is evaluated later.

**Variable Accuracy:**

Obviously, LAMMPS attempts to evaluate variables containing formulas (equal and atom style variables) accurately whenever the evaluation is performed. Depending on what is included in the formula, this may require invoking a compute, either directly or indirectly via a thermo keyword, or accessing a value previously calculated by a compute, or accessing a value calculated and stored by a fix. If the compute is one that calculates the pressure or energy of the system, then these quantities need to be tallied during the evaluation of the interatomic potentials (pair, bond, etc) on timesteps that the variable will need the values.

LAMMPS keeps track of all of this during a run or energy minimization. An error will be generated if you attempt to evaluate a variable on timesteps when it cannot produce accurate values. For example, if a thermo_style custom command prints a variable which accesses values stored by a fix ave/time command and the timesteps on which thermo output is generated are not multiples of the averaging frequency used in the fix command, then an error will occur.

An input script can also request variables be evaluated before or after or in between runs, e.g. by including them in a print command. In this case, if a compute is needed to evaluate a variable (either directly or indirectly), LAMMPS will not invoke the compute, but it will use a value previously calculated by the compute, and can do this only if it is current. Fixes will always provide a quantity needed by a variable, but the quantity may or may
not be current. This leads to one of three kinds of behavior:

(1) The variable may be evaluated accurately. If it contains references to a compute or fix, and these values were calculated on the last timestep of a preceding run, then they will be accessed and used by the variable and the result will be accurate.

(2) LAMMPS may not be able to evaluate the variable and generate an error. For example, if the variable requires a quantity from a compute that is not current, LAMMPS will generate an error. This means, for example, that such a variable cannot be evaluated before the first run has occurred. Likewise, in between runs, such a variable cannot be accessed unless it was evaluated on the last timestep of the preceding run, e.g. by thermodynamic output.

One way to get around this problem is to perform a 0-timestep run before using the variable. For example, these commands

variable t equal temp
print "Initial temperature = $t"
run 1000

will generate an error if the run is the first run specified in the input script, because generating a value for the "t" variable requires a compute for calculating the temperature to be invoked.

However, this sequence of commands would be fine:

run 0
variable t equal temp
print "Initial temperature = $t"
run 1000

The 0-timestep run initializes and invokes various computes, including the one for temperature, so that the value it stores is current and can be accessed by the variable "t" after the run has completed. Note that a 0-timestep run does not alter the state of the system, so it does not change the input state for the 1000-timestep run that follows. Also note that the 0-timestep run must actually use and invoke the compute in question (e.g. via thermo or dump output) in order for it to enable the compute to be used in a variable after the run. Thus if you are trying to print a variable that uses a compute you have defined, you could insure it was invoked on the last timestep of the preceding run by including it in thermodynamic output.

Unlike computes, fixes will never generate an error if their values are accessed by a variable in between runs. They always return some value to the variable. However, the value may not be what you expect if the fix has not yet calculated the quantity of interest or it is not current. For example, the fix indent command stores the force on the indenter. But this is not computed until a run is performed. Thus if a variable attempts to print this value before the first run, zeroes will be output. Again, performing a 0-timestep run before printing the variable has the desired effect.

(3) The variable may be evaluated incorrectly. And LAMMPS may have no way to detect this has occurred. Consider the following sequence of commands:

pair_coeff 1 1 1.0 1.0
run 1000
pair_coeff 1 1 1.5 1.0
variable e equal pe
print "Final potential energy = $e"

The first run is performed using one setting for the pairwise potential defined by the pair_style and pair_coeff commands. The potential energy is evaluated on the final timestep and stored by the compute pe compute (this is
done by the `thermo_style` command). Then a pair coefficient is changed, altering the potential energy of the system. When the potential energy is printed via the "$e" variable, LAMMPS will use the potential energy value stored by the `compute pe` compute, thinking it is current. There are many other commands which could alter the state of the system between runs, causing a variable to evaluate incorrectly.

The solution to this issue is the same as for case (2) above, namely perform a 0-timestep run before the variable is evaluated to insure the system is up-to-date. For example, this sequence of commands would print a potential energy that reflected the changed pairwise coefficient:

```
pair_coeff 1 1 1.0 1.0
run 1000
pair_coeff 1 1 1.5 1.0
run 0
variable e equal pe
print "Final potential energy = $e"
```

**Restrictions:**

Indexing any formula element by global atom ID, such as an atom value, requires the atom style to use a global mapping in order to look up the vector indices. By default, only atom styles with molecular information create global maps. The `atom_modify map` command can override the default.

All `universe`- and `uloop`-style variables defined in an input script must have the same number of values.

**Related commands:**

`next, jump, include, temper, fix print, print`

**Default:** none
velocity command

Syntax:

velocity group-ID style args keyword value ...

- **group-ID** = ID of group of atoms whose velocity will be changed
- **style** = *create* or *set* or *scale* or *ramp* or *zero*

```plaintext
create args = temp seed
  temp = temperature value (temperature units)
  seed = random # seed (positive integer)
set args = vx vy vz
  vx, vy, vz = velocity value or NULL (velocity units)
  any of vx, vy, vz can be a variable (see below)
scale args = temp
  temp = temperature value (temperature units)
ramp args = vdim vlo vhi dim clo chi
  vdim = vx or vy or vz
  vlo, vhi = lower and upper velocity value (velocity units)
  dim = x or y or z
  clo, chi = lower and upper coordinate bound (distance units)
zero args = linear or angular
  linear = zero the linear momentum
  angular = zero the angular momentum
```

- zero or more keyword/value pairs may be appended
- **keyword** = *dist* or *sum* or *mom* or *rot* or *temp* or *loop* or *units*

```plaintext
dist value = uniform or gaussian
  sum value = no or yes
  mom value = no or yes
  rot value = no or yes
  temp value = temperature ID
  loop value = all or local or geom
  units value = box or lattice
```

Examples:

```plaintext
velocity all create 300.0 4928459 rot yes dist gaussian
velocity border set NULL 4.0 v_vz sum yes units box
velocity flow scale 300.0
velocity flow ramp vx 0.0 5.0 y 5 25 temp mytemp
velocity all zero linear
```

Description:

Set or change the velocities of a group of atoms in one of several styles. For each style, there are required arguments and optional keyword/value parameters. Not all options are used by each style. Each option has a default as listed below.

The *create* style generates an ensemble of velocities using a random number generator with the specified seed as the specified temperature.

The *set* style sets the velocities of all atoms in the group to the specified values. If any component is specified as NULL, then it is not set. Any of the vx, vy, vz velocity components can be specified as an equal-style or atom-style
variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated, and its value used to determine the velocity component.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters or other parameters.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent velocity field.

The scale style computes the current temperature of the group of atoms and then rescales the velocities to the specified temperature.

The ramp style is similar to that used by the compute temp/ramp command. Velocities ramped uniformly from vlo to vhi are applied to dimension vx, or vy, or vz. The value assigned to a particular atom depends on its relative coordinate value (in dim) from clo to chi. For the example above, an atom with y-coordinate of 10 (1/4 of the way from 5 to 25), would be assigned a x-velocity of 1.25 (1/4 of the way from 0.0 to 5.0). Atoms outside the coordinate bounds (less than 5 or greater than 25 in this case), are assigned velocities equal to vlo or vhi (0.0 or 5.0 in this case).

The zero style adjusts the velocities of the group of atoms so that the aggregate linear or angular momentum is zero. No other changes are made to the velocities of the atoms.

All temperatures specified in the velocity command are in temperature units; see the units command. The units of velocities and coordinates depend on whether the units keyword is set to box or lattice, as discussed below.

For all styles, no atoms are assigned z-component velocities if the simulation is 2d; see the dimension command.

The keyword/value option pairs are used in the following ways by the various styles.

The dist option is used by create. The ensemble of generated velocities can be a uniform distribution from some minimum to maximum value, scaled to produce the requested temperature. Or it can be a gaussian distribution with a mean of 0.0 and a sigma scaled to produce the requested temperature.

The sum option is used by all styles, except zero. The new velocities will be added to the existing ones if sum = yes, or will replace them if sum = no.

The mom and rot options are used by create. If mom = yes, the linear momentum of the newly created ensemble of velocities is zeroed; if rot = yes, the angular momentum is zeroed.

The temp option is used by create and scale to specify a compute that calculates temperature in a desired way. If this option is not specified, create and scale calculate temperature using a compute that is defined as follows:

compute velocity_temp group-ID temp

where group-ID is the same ID used in the velocity command. i.e. the group of atoms whose velocity is being altered. This compute is deleted when the velocity command is finished. See the compute temp command for details. If the computed temperature should have degrees-of-freedom removed due to fix constraints (e.g. SHAKE or rigid-body constraints), then the appropriate fix command must be specified before the velocity command is issued.

The loop option is used by create in the following ways.
If loop = all, then each processor loops over all atoms in the simulation to create velocities, but only stores velocities for atoms it owns. This can be a slow loop for a large simulation. If atoms were read from a data file, the velocity assigned to a particular atom will be the same, independent of how many processors are being used. This will not be the case if atoms were created using the create_atoms command, since atom IDs will likely be assigned to atoms differently.

If loop = local, then each processor loops over only its atoms to produce velocities. The random number seed is adjusted to give a different set of velocities on each processor. This is a fast loop, but the velocity assigned to a particular atom will depend on which processor owns it. Thus the results will always be different when a simulation is run on a different number of processors.

If loop = geom, then each processor loops over only its atoms. For each atom a unique random number seed is created, based on the atom's xyz coordinates. A velocity is generated using that seed. This is a fast loop and the velocity assigned to a particular atom will be the same, independent of how many processors are used. However, the set of generated velocities may be more correlated than if the all or local options are used.

Note that the loop geom option will not necessarily assign identical velocities for two simulations run on different machines. This is because the computations based on xyz coordinates are sensitive to tiny differences in the double-precision value for a coordinate as stored on a particular machine.

The units option is used by set and ramp. If units = box, the velocities and coordinates specified in the velocity command are in the standard units described by the units command (e.g. Angstroms/fmsec for real units). If units = lattice, velocities are in units of lattice spacings per time (e.g. spacings/fmsec) and coordinates are in lattice spacings. The lattice command must have been previously used to define the lattice spacing.

Restrictions: none

Related commands: fix shake, lattice

Default:

The option defaults are dist = uniform, sum = no, mom = yes, rot = no, temp = full style on group-ID, loop = all, and units = lattice.
write_restart command

Syntax:

write_restart file

- file = name of file to write restart information to

Examples:

write_restart restart.equil
write_restart poly.%.*

Description:

Write a binary restart file of the current state of the simulation. See the read_restart command for information about what is stored in a restart file.

During a long simulation, the restart command is typically used to dump restart files periodically. The write_restart command is useful after a minimization or whenever you wish to write out a single current restart file.

Similar to dump files, the restart filename can contain two wild-card characters. If a "#" appears in the filename, it is replaced with the current timestep value. If a "%" character appears in the filename, then one file is written by each processor and the "%" character is replaced with the processor ID from 0 to P-1. An additional file with the "%" replaced by "base" is also written, which contains global information. For example, the files written for filename restart.% would be restart.base, restart.0, restart.1, ... restart.P-1. This creates smaller files and can be a fast mode of output and subsequent input on parallel machines that support parallel I/O.

Restart files can be read by a read_restart command to restart a simulation from a particular state. Because the file is binary (to enable exact restarts), it may not be readable on another machine. In this case, the restart2data program in the tools directory can be used to convert a restart file to an ASCII data file. Both the read_restart command and restart2data tool can read in a restart file that was written with the "%" character so that multiple files were created.

Restrictions:

This command requires inter-processor communication to migrate atoms before the restart file is written. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses initialized, etc).

Related commands:

restart, read_restart

Default: none