

## ERRORS

These doc pages describe many of the error and warning message you can encounter when using LAMMPS. The common problems include conceptual issues. The messages and warnings doc pages give complete lists of all the messages the code may generate, with additional details for many of them.

### 11.1 Common problems

If two LAMMPS runs do not produce the exact 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 thermostating.

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. For most errors it will also print the last input script command that it was processing. 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 does not catch that you think it should flag, please send an email to the [developers](#) or create a new topic on the dedicated [MatSci forum section](#).

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. If you get an error like “Invalid ... style”, with ... being fix, compute, pair, etc, it means that you mistyped the style name or that the command is part of an optional package which was not compiled into your executable. The list of available styles in your executable can be listed by using *the -h command-line switch*. The installation and compilation of optional packages is explained on the [Build packages](#) doc page.

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 also simply 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 of 0. Careful reading of the associated doc page for the

command should allow you to fix these problems. In most cases, where LAMMPS expects to read a number, either integer or floating point, it performs a stringent test on whether the provided input actually is an integer or floating-point number, respectively, and reject the input with an error message (for instance, when an integer is required, but a floating-point number 1.0 is provided):

ERROR: Expected integer parameter instead of '1.0' in input script or data file

Some commands allow for using variable references in place of numeric constants so that the value can be evaluated and may change over the course of a run. This is typically done with the syntax `v_name` for a parameter, where name is the name of the variable. On the other hand, immediate variable expansion with the syntax `${name}` is performed while reading the input and before parsing commands,

#### **Note**

Using a variable reference (i.e. `v_name`) is only allowed if the documentation of the corresponding command explicitly says it is. Otherwise, you will receive an error message of this kind:

ERROR: Expected floating point parameter instead of 'v\_name' in input script or data file

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 should not 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 does not 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 ensure 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.

## 11.2 Error and warning details

Many errors or warnings are self-explanatory and thus straightforward to resolve. However, there are also cases, where there is no single cause and explanation, where LAMMPS can only detect symptoms of an error but not the exact cause, or where the explanation needs to be more detailed than what can be fit into a message printed by the program. The following are discussions of such cases.

### 11.2.1 Unknown identifier in data file

This error happens when LAMMPS encounters a line of text with an unexpected keyword while *reading a data file*. This would be either header keywords or section header keywords. This is most commonly due to a mistyped keyword or due to a keyword that is inconsistent with the *atom style* used.

The header section informs LAMMPS how many entries or lines are expected in the various sections (like Atoms, Masses, Pair Coeffs, *etc.*) of the data file. If there is a mismatch, LAMMPS will either keep reading beyond the end of a section or stop reading before the section has ended. In that case the next line will not contain a recognized keyword.

Such a mismatch can also happen when the first line of the data is *not* a comment as required by the format, but a line with a valid header keyword. That would result in LAMMPS expecting, for instance, 0 atoms because the “atoms” header line is the first line and thus treated as a comment.

Another possibility to trigger this error is to have a keyword in the data file that corresponds to a fix (e.g. *fix cmap*) but the *read\_data* command is missing the (optional) arguments that identify the fix and the header keyword and section keyword or those arguments are inconsistent with the keywords in the data file.

### 11.2.2 Incorrect format in ... section of data file

This error happens when LAMMPS reads the contents of a section of a *data file* and the number of parameters in the line differs from what is expected. This most commonly happens, when the atom style is different from what is expected for a specific data file since changing the atom style usually changes the format of the line.

This error can also happen when the number of entries indicated in the header of a data file (e.g. the number of atoms) is larger than the number of lines provided (e.g. in the corresponding Atoms section) and then LAMMPS will continue reading into the next section and that would have a completely different format.

## 11.3 Reporting bugs

If you are confident that you have found a bug in LAMMPS, please follow the steps outlined below:

- Check the [New features and bug fixes](#) section of the [LAMMPS WWW site](#) or the [GitHub Releases page](#) to see if the bug has already been addressed in a patch release.
- Check that your issue can be reproduced with the latest development version of LAMMPS.
- Check the manual carefully to verify that the unexpected behavior you are observing is indeed in conflict with the documentation
- Check the [GitHub Issue page](#) if your issue has already been reported and if it is still open.
- Check the [GitHub Pull Requests page](#) to see if there is already a fix for your bug pending.
- Check the [LAMMPS forum at MatSci](#) to see if the issue has been discussed before.

If none of these steps yields any useful information, please file a new bug report on the [GitHub Issue page](#). The website will offer you to select a suitable template with explanations and then you should replace those explanations with the information that you can provide to reproduce your issue.

The most useful thing you can do to help us verify and fix a bug is to isolate the problem. Run it on the smallest number of atoms and fewest number of processors with the simplest input script that reproduces the bug. Try to identify what command or combination of commands is causing the problem and upload the complete input deck as a tar or zip archive. Please avoid using binary restart files unless the issue requires it. In the latter case you should also include an input deck to quickly generate this restart from a data file or a simple additional input. This input deck can be used with tools like a debugger or *valgrind* to further *debug the crash*.

You may also post a message in the [development category](#) of the LAMMPS forum at [MatSci](#) describing the problem with the same kind of information. The forum can provide a faster response, especially if the bug reported is actually expected behavior or other LAMMPS users have come across it before.

## 11.4 Debugging crashes

If LAMMPS crashes with a “segmentation fault” or a “bus error” or similar message, then you can use the following two methods to further narrow down the origin of the issue. This will help the LAMMPS developers (or yourself) to understand the reason for the crash and apply a fix (either to the input script or the source code). This requires that your LAMMPS executable includes the required [debug information](#). Otherwise it is not possible to look up the names of functions or variables.

The following patch will introduce a bug into the code for pair style *lj/cut* when using the examples/melt/in.melt input. We use it to show how to identify the origin of a segmentation fault.

```
--- a/src/pair_lj_cut.cpp
+++ b/src/pair_lj_cut.cpp
@@ -81,6 +81,7 @@ void PairLJCut::compute(int eflag, int vflag)
    int nlocal = atom->nlocal;
    double *special_lj = force->special_lj;
    int newton_pair = force->newton_pair;
+   double comx = 0.0;

    inum = list->inum;
    ilist = list->ilist;
@@ -134,8 +135,10 @@ void PairLJCut::compute(int eflag, int vflag)
        evdwl,0.0,fpair,dex,dely,dely);
    }
- }
+ }

+   comx += atom->rmas[i]*x[i][0]; /* BUG */
+ }
+   printf("comx = %g\n",comx);
    if (vflag_fdotr) virial_fdotr_compute();
}
```

After recompiling LAMMPS and running the input you should get something like this:

```
$ ./lmp -in in.melt
LAMMPS (19 Mar 2020)
  using 1 OpenMP thread(s) per MPI task
Lattice spacing in x,y,z = 1.6796 1.6796 1.6796
Created orthogonal box = (0 0 0) to (16.796 16.796 16.796)
  1 by 1 by 1 MPI processor grid
Created 4000 atoms
  create_atoms CPU = 0.000432253 secs
Neighbor list info ...
  update every 20 steps, delay 0 steps, check no
  max neighbors/atom: 2000, page size: 100000
  master list distance cutoff = 2.8
  ghost atom cutoff = 2.8
```

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```

binsize = 1.4, bins = 12 12 12
1 neighbor lists, perpetual/occasional/extra = 1 0 0
(1) pair lj/cut, perpetual
  attributes: half, newton on
  pair build: half/bin/atomonly/newton
  stencil: half/bin/3d/newton
  bin: standard
Setting up Verlet run ...
Unit style    : lj
Current step  : 0
Time step     : 0.005
Segmentation fault (core dumped)

```

### 11.4.1 Using the GDB debugger to get a stack trace

There are two options to use the GDB debugger for identifying the origin of the segmentation fault or similar crash. The GDB debugger has many more features and options, as can be seen for example its [online documentation](#).

#### Run LAMMPS from within the debugger

Running LAMMPS under the control of the debugger as shown below only works for a single MPI rank (for debugging a program running in parallel you usually need a parallel debugger program). A simple way to launch GDB is to prefix the LAMMPS command line with `gdb --args` and then type the command “run” at the GDB prompt. This will launch the debugger, load the LAMMPS executable and its debug info, and then run it. When it reaches the code causing the segmentation fault, it will stop with a message why it stopped, print the current line of code, and drop back to the GDB prompt.

```

(gdb) run
[...]
Setting up Verlet run ...
Unit style    : lj
Current step  : 0
Time step     : 0.005

Program received signal SIGSEGV, Segmentation fault.
0x00000000006653ab in LAMMPS_NS::PairLJCut::compute (this=0x829740, eflag=1, vflag=<optimized out>) at /home/akohlmey/compile/lammps/src/pair_lj_cut.cpp:139
139      comx += atom->rmas[i]*x[i][0]; /* BUG */
(gdb)

```

Now typing the command “where” will show the stack of functions starting from the current function back to “main()”.

```

(gdb) where
#0  0x00000000006653ab in LAMMPS_NS::PairLJCut::compute (this=0x829740, eflag=1, vflag=<optimized out>) at /home/akohlmey/compile/lammps/src/pair_lj_cut.cpp:139
#1  0x00000000004cf0a2 in LAMMPS_NS::Verlet::setup (this=0x7e6c90, flag=1) at /home/akohlmey/compile/lammps/src/verlet.cpp:131
#2  0x000000000049db42 in LAMMPS_NS::Run::command (this=this@entry=0x7ffffffcca0, narg=narg@entry=1, arg=arg@entry=0x7e8750) at /home/akohlmey/compile/lammps/src/run.cpp:177

```

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```
#3 0x00000000041258a in LAMMPS_NS::Input::command_creator<LAMMPS_NS::Run> (lmp=
→<optimized out>, nargs=1, arg=0x7e8750)
   at /home/akohlmey/compile/lammps/src/input.cpp:878
#4 0x000000000410ad3 in LAMMPS_NS::Input::execute_command (this=0x7d1410) at /home/
→akohlmey/compile/lammps/src/input.cpp:864
#5 0x0000000004111fb in LAMMPS_NS::Input::file (this=0x7d1410) at /home/akohlmey/compile/
→lammps/src/input.cpp:229
#6 0x00000000040933a in main (argc=<optimized out>, argv=<optimized out>) at /home/akohlmey/
→compile/lammps/src/main.cpp:65
(gdb)
```

You can also print the value of variables and see if there is anything unexpected. Segmentation faults, for example, commonly happen when a pointer variable is not assigned and still initialized to NULL.

```
(gdb) print x
$1 = (double **) 0x7fff7ca1010
(gdb) print i
$2 = 0
(gdb) print x[0]
$3 = (double *) 0x7fff6d80010
(gdb) print x[0][0]
$4 = 0
(gdb) print x[1][0]
$5 = 0.83979809569125363
(gdb) print atom->rmas
$6 = (double *) 0x0
(gdb)
```

### Inspect a core dump file with the debugger

When an executable crashes with a “core dumped” message, it creates a file “core” or “core.<PID#>” which contains the information about the current state. This file may be located in the folder where you ran LAMMPS or in some hidden folder managed by the systemd daemon. In the latter case, you need to “extract” the core file with the `coredumpctl` utility to the current folder. Example: `coredumpctl -o core dump lmp`. Now you can launch the debugger to load the executable, its debug info and the core dump and drop you to a prompt like before.

```
$ gdb lmp core
Reading symbols from lmp...
[New LWP 1928535]
[Thread debugging using libthread_db enabled]
Using host libthread_db library "/lib64/libthread_db.so.1".
Core was generated by `./lmp -in in.melt'.
Program terminated with signal SIGSEGV, Segmentation fault.
#0 0x00000000006653ab in LAMMPS_NS::PairLJCut::compute (this=0x1b10740, eflag=1, vflag=
→<optimized out>)
   at /home/akohlmey/compile/lammps/src/pair_lj_cut.cpp:139
139     comx += atom->rmas[i]*x[i][0]; /* BUG */
(gdb)
```

From here on, you use the same commands as shown before to get a stack trace and print current values of (pointer) variables.

### 11.4.2 Using valgrind to get a stack trace

The `valgrind` suite of tools allows to closely inspect the behavior of a compiled program by essentially emulating a CPU and instrumenting the program while running. This slows down execution quite significantly, but can also report issues that are not resulting in a crash. The default valgrind tool is a memory checker and you can use it by prefixing the normal command line with `valgrind`. Unlike GDB, this will also work for parallel execution, but it is recommended to redirect the valgrind output to a file (e.g. with `--log-file=crash-%p.txt`, the `%p` will be substituted with the process ID) so that the messages of the multiple valgrind instances to the console are not mixed.

```
$ valgrind ./lmp -in in.melt
==1933642== Memcheck, a memory error detector
==1933642== Copyright (C) 2002-2017, and GNU GPL'd, by Julian Seward et al.
==1933642== Using Valgrind-3.15.0 and LibVEX; rerun with -h for copyright info
==1933642== Command: ./lmp -in in.melt
==1933642==
LAMMPS (19 Mar 2020)
OMP_NUM_THREADS environment is not set. Defaulting to 1 thread. (src/comm.cpp:94)
  using 1 OpenMP thread(s) per MPI task
Lattice spacing in x,y,z = 1.6796 1.6796 1.6796
Created orthogonal box = (0 0 0) to (16.796 16.796 16.796)
  1 by 1 by 1 MPI processor grid
Created 4000 atoms
  create_atoms CPU = 0.032964 secs
Neighbor list info ...
  update every 20 steps, delay 0 steps, check no
  max neighbors/atom: 2000, page size: 100000
  master list distance cutoff = 2.8
  ghost atom cutoff = 2.8
  binsize = 1.4, bins = 12 12 12
  1 neighbor lists, perpetual/occasional/extra = 1 0 0
  (1) pair lj/cut, perpetual
    attributes: half, newton on
    pair build: half/bin/atomonly/newton
    stencil: half/bin/3d/newton
    bin: standard
Setting up Verlet run ...
  Unit style   : lj
  Current step : 0
  Time step    : 0.005
==1933642== Invalid read of size 8
==1933642== at 0x6653AB: LAMMPS_NS::PairLJCut::compute(int, int) (pair_lj_cut.cpp:139)
==1933642== by 0x4CF0A1: LAMMPS_NS::Verlet::setup(int) (verlet.cpp:131)
==1933642== by 0x49DB41: LAMMPS_NS::Run::command(int, char**) (run.cpp:177)
==1933642== by 0x412589: void LAMMPS_NS::Input::command_creator<LAMMPS_NS::Run>
→(LAMMPS_NS::LAMMPS*, int, char**) (input.cpp:881)
==1933642== by 0x410AD2: LAMMPS_NS::Input::execute_command() (input.cpp:864)
==1933642== by 0x4111FA: LAMMPS_NS::Input::file() (input.cpp:229)
==1933642== by 0x409339: main (main.cpp:65)
==1933642== Address 0x0 is not stack'd, malloc'd or (recently) free'd
==1933642==
```

As you can see, the stack trace information is similar to that obtained from GDB. In addition you get a more specific hint about what cause the segmentation fault, i.e. that it is a NULL pointer dereference. To find out which pointer exactly was NULL, you need to use the debugger, though.



## 11.5 Error messages

This is an alphabetic list of the ERROR messages LAMMPS prints out and the reason why. If the explanation here is not sufficient, the documentation for the offending command may help. Error messages also list the source file and line number where the error was generated. For example, a message like this:

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.

Doc page with [WARNING messages](#)

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### ***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.

### ***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 atom IDs = 0 but atom\_modify id = yes***

Self-explanatory.

### ***All atoms of a swapped type must have same charge.***

Self-explanatory.

### ***All atoms of a swapped type must have the same charge.***

Self-explanatory.

### ***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 mol IDs should be set for fix gcmc group atoms***

The molecule flag is on, yet not all molecule ids in the fix group have been set to non-zero positive values by the user. This is an error since all atoms in the fix gcmc group are eligible for deletion, rotation, and translation and therefore must have valid molecule ids.

### ***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 three 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 atoms missing on proc %d at step %ld***

One or more of three 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 extent > half of periodic box length***

This error was detected by the neigh\_modify check yes setting. It is an error because the angle atoms are so far apart it is ambiguous how it should be defined.

***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 angle 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.

***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 body parameters to non-body atom***

Self-explanatory.

***Assigning ellipsoid parameters to non-ellipsoid atom***

Self-explanatory.

***Assigning line parameters to non-line atom***

Self-explanatory.

***Assigning quat to non-body atom***

Self-explanatory.

***Assigning tri parameters to non-tri atom***

Self-explanatory.

***At least one atom of each swapped type must be present to define charges.***

Self-explanatory.

***Atom IDs must be consecutive for velocity create loop all***

Self-explanatory.

***Atom IDs must be used for molecular systems***

Atom IDs are used to identify and find partner atoms in bonds.

***Atom count changed in fix neb***

This is not allowed in a NEB calculation.

***Atom count is inconsistent, cannot write data file***

The sum of atoms across processors does not equal the global number of atoms. Probably some atoms have been lost.

***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 style hybrid cannot have hybrid as an argument***

Self-explanatory.

***Atom style hybrid cannot use same atom style twice***

Self-explanatory.

***Atom style template molecule must have atom types***

The defined molecule(s) does not specify atom types.

***Atom style was redefined after using fix property/atom***

This is not allowed.

***Atom type must be zero in fix gcmc mol command***

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 id command after simulation box is defined***

The atom\_modify id command cannot be used after a read\_data, read\_restart, or create\_box command.

***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.

***Atomfile variable could not read values***

Check the file assigned to the variable.

***Atomfile variable in equal-style variable formula***

Self-explanatory.

***Atomfile-style variable in equal-style variable formula***

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.

***Attempting to insert more particles than available lattice points***

Self-explanatory.

***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 angle type for PPPMDisp/TIP4P***

Specified angle type is not valid.

***Bad TIP4P bond type for PPPM/TIP4P***

Specified bond type is not valid.

***Bad TIP4P bond type for PPPMDisp/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 “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 kmax/ewald parameter***

Kspace\_modify values for the kmax/ewald keyword must be integers > 0

***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.

***Bad real space Coulombic cutoff in fix tune/kspace***

Fix tune/kspace tried to find the optimal real space Coulombic cutoff using the Newton-Rhaphson method, but found a non-positive or NaN cutoff

***Balance command before simulation box is defined***

The balance command cannot be used before a read\_data, read\_restart, or create\_box command.

***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.

***Balance rcb cannot be used with comm\_style brick***

Comm\_style tiled must be used instead.

***Balance shift string is invalid***

The string can only contain the characters “x”, “y”, or “z”.

***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 spheroids 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***

Format of bigint stored in restart file is not consistent with LAMMPS version you are running. See the settings in src/lmptype.h

***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 second atom 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 image check***

The second atom in 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 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***

The second atom 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 atoms missing on proc %d at step %ld***

The second atom 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 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 extent > half of periodic box length***

This error was detected by the neigh\_modify check yes setting. It is an error because the bond atoms are so far apart it is ambiguous how it should be defined.

***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 bond 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 cannot be used with atom style template***

This bond style can change the bond topology which is not allowed with this atom style.

***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.

***BondAngle coeff for hybrid angle has invalid format***

No “ba” field should appear in data file entry.

***BondBond coeff for hybrid angle has invalid format***

No “bb” field should appear in data file entry.

***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 restart files must use % or neither***

Self-explanatory.

***Both restart files must use MPI-IO or neither***

Self-explanatory.

***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.

***Box command after simulation box is defined***

The box command cannot be used after a read\_data, read\_restart, or create\_box command.

***CPU neighbor lists must be used for ellipsoid/sphere mix.***

When using Gay-Berne or RE-squared pair styles with both ellipsoidal and spherical particles, the neighbor list must be built on the CPU

***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 page discussion of command-line switches.

***Can only use -pscreen with multiple partitions***

Self-explanatory. See page discussion of command-line switches.

***Can only use Kokkos supported regions with Kokkos package***

Self-explanatory.

***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) do analytic differentiation with pppm/gpu***

This is a current restriction of this command.

***Cannot (yet) request ghost atoms with Kokkos half neighbor list***

This feature is not yet supported.

***Cannot (yet) use 'electron' units with dipoles***

This feature is not yet supported.

***Cannot (yet) use Ewald with triclinic box and slab correction***

This feature is not yet supported.

***Cannot (yet) use K-space slab correction with compute group/group for triclinic systems***

This option is not yet supported.

***Cannot (yet) use MSM with 2d simulation***

This feature is not yet supported.

***Cannot (yet) use PPPM with triclinic box and TIP4P***

This feature is not yet supported.

***Cannot (yet) use PPPM with triclinic box and kspace\_modify diff ad***

This feature is not yet supported.

***Cannot (yet) use PPPM with triclinic box and slab correction***

This feature is not yet supported.

***Cannot (yet) use kspace slab correction with long-range dipoles and non-neutral systems or per-atom energy***

This feature is not yet supported.

***Cannot (yet) use kspace\_modify diff ad with compute group/group***

This option is not yet supported.

***Cannot (yet) use kspace\_style pppm/stagger with triclinic systems***

This feature is not yet supported.



***Cannot (yet) use molecular templates with Kokkos***

Self-explanatory.

***Cannot (yet) use respa with Kokkos***

Self-explanatory.

***Cannot (yet) use rigid bodies with fix deform and Kokkos***

Self-explanatory.

***Cannot (yet) use rigid bodies with fix nh and Kokkos***

Self-explanatory.

***Cannot (yet) use single precision with MSM (remove -DFFT\_SINGLE from Makefile and re-compile)***

Single precision cannot be used with MSM.

***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 non-periodic 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 is because fix pour pre-computes the time delay for particles to fall out of the insertion volume due to gravity.

***Cannot change to comm\_style brick from tiled layout***

Self-explanatory.

***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 clear group all***

This operation is not allowed.

***Cannot close restart file - MPI error: %s***

This error was generated by MPI when reading/writing an MPI-IO restart file.

***Cannot compute initial g\_ewald\_disp***

LAMMPS failed to compute an initial guess for the PPPM\_disp g\_ewald\_6 factor that partitions the computation between real space and k-space for Dispersion interactions.

***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 allocators, 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***

A simulation box can only be defined once.

***Cannot currently use pair reax with pair hybrid***

This is not yet supported.

***Cannot currently use pppm/gpu with fix balance.***

Self-explanatory.

***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 delete\_atoms bond yes for non-molecular systems***

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 do atom/swap 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 sort on atom IDs with no atom IDs defined***

Self-explanatory.

***Cannot dump sort when multiple dump files are written***

In this mode, each processor dumps its atoms to a file, so no sorting is allowed.

***Cannot embed Python when also extending Python with LAMMPS***

When running LAMMPS via Python through the LAMMPS library interface you cannot also use the input script python command.

***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 create\_bonds group ID***

Self-explanatory.

***Cannot find delete\_bonds group ID***

Group ID used in the delete\_bonds command does not exist.

***Cannot find specified group ID for core particles***

Self-explanatory.

***Cannot find specified group ID for shell particles***

Self-explanatory.

***Cannot have both pair\_modify shift and tail set to yes***

These 2 options are contradictory.

***Cannot intersect groups using a dynamic group***

This operation is not allowed.

***Cannot mix molecular and molecule template atom styles***

Self-explanatory.

***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 COMB3 lib.comb3 file***

The COMB3 library file cannot be opened. Check that the path and name are correct.

***Cannot open COMB3 potential file %s***

The specified COMB3 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 SNAP coefficient file %s***

The specified SNAP coefficient file cannot be opened. Check that the path and name are correct.

***Cannot open SNAP parameter file %s***

The specified SNAP parameter 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 potential file cannot be opened. Check that the path and name are correct.

***Cannot open Vashishta potential file %s***

The specified Vashishta potential file cannot be opened. Check that the path and name are correct.

***Cannot open balance output file***

Self-explanatory.

***Cannot open coul/streitz potential file %s***

The specified coul/streitz potential file cannot be opened. Check that the path and name are correct.

***Cannot open custom file***

Self-explanatory.

***Cannot open data file %s***

The specified file cannot be opened. Check that the path and name are correct.

***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***

Self-explanatory.

***Cannot open dump file %s***

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. If the file is a compressed file, also check that the gzip executable can be found and run.

***Cannot open file variable file %s***

The specified file cannot be opened. Check that the path and name are correct.

***Cannot open fix ave/chunk 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/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 parameter file %s***

The specified file cannot be opened. Check that the path and name are correct.

***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 rigid restart file %s***

The specified file cannot be opened. Check that the path and name are correct.

***Cannot open fix rigid/small 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 was compiled without support for reading and writing gzipped files through a pipeline to the gzip program with -DLAMMPS\_GZIP.

***Cannot open input script %s***

Self-explanatory.

***Cannot open log.cite file***

This file is created when you use some LAMMPS features, to indicate what paper you should cite on behalf of those who implemented the feature. Check that you have write privileges into the directory you are running in.

***Cannot open log.lammps for writing***

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 molecule file %s***

The specified file cannot be opened. Check that the path and name are correct.

***Cannot open nb3b/harmonic potential file %s***

The specified potential file 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 polymorphic potential file %s***

The specified polymorphic potential file cannot be opened. Check that the path and name are correct.

***Cannot open print file %s***

Self-explanatory.

***Cannot open processors output file***

Self-explanatory.

***Cannot open restart file %s***

Self-explanatory.

***Cannot open restart file for reading - MPI error: %s***

This error was generated by MPI when reading/writing an MPI-IO restart file.

***Cannot open restart file for writing - MPI error: %s***

This error was generated by MPI when reading/writing an MPI-IO restart file.

***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 temporary file for world counter.***

Self-explanatory.

***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 from restart file - MPI error: %s***

This error was generated by MPI when reading/writing an MPI-IO restart file.

***Cannot read\_data without add keyword after simulation box is defined***

Self-explanatory.

***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 run 2d simulation with non-periodic Z dimension***

Use the boundary command to make the z dimension periodic in order to run a 2d simulation.

***Cannot set bond topology types for atom style template***

The bond, angle, etc types cannot be changed for this atom style since they are static settings in the molecule template files.

***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 cutoff/multi before simulation box is defined***

Self-explanatory.

***Cannot set dpd/theta for this atom style***

Self-explanatory.

***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/cv for this atom style***

Self-explanatory.

***Cannot set meso/e for this atom style***

Self-explanatory.

***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 quaternion with xy components for 2d system***

Self-explanatory.

***Cannot set respa hybrid and any of pair/inner/middle/outer***

In the rRESPA integrator, you must compute pairwise potentials either all together (pair), with different cutoff regions (inner/middle/outer), or per hybrid sub-style (hybrid). You cannot mix those.

***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 restart file size - MPI error: %s***

This error was generated by MPI when reading/writing an MPI-IO restart file.

***Cannot set smd/contact/radius for this atom style***

Self-explanatory.

***Cannot set smd/mass/density for this atom style***

Self-explanatory.

***Cannot set temperature for fix rigid/nph***

The temp keyword cannot be specified.

***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 subtract groups using a dynamic group***

This operation is not allowed.

***Cannot union groups using a dynamic group***

This operation is not allowed.

***Cannot use -kokkos on without KOKKOS installed***

Self-explanatory.

***Cannot use -reorder after -partition***

Self-explanatory. See 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/disp solver on system with no charge, dipole, or LJ particles***

No atoms in system have a non-zero charge or dipole, or are LJ particles. Change charges/dipoles or change options of the kspace solver/pair style.

***Cannot use EwaldDisp with 2d simulation***

This is a current restriction of this command.

***Cannot use Kokkos pair style with rRESPA inner/middle***

Self-explanatory.

***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 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 PPPMDisp with 2d simulation***

The kspace style ppm/disp cannot be used in 2d simulations. You can use 2d ppm/disp in a 3d simulation; see the kspace\_modify command.

***Cannot use PRD with a changing box***

The current box dimensions are not copied between replicas

***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 atomfile-style variable unless atom map exists***

Self-explanatory. See the atom\_modify command to create a map.

***Cannot use both com and bias with compute temp/chunk***

Self-explanatory.

***Cannot use chosen neighbor list style with buck/coul/cut/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with buck/coul/long/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with buck/kk***

That style is not supported by Kokkos.

***Cannot use chosen neighbor list style with coul/cut/kk***

That style is not supported by Kokkos.

***Cannot use chosen neighbor list style with coul/debye/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with coul/dsf/kk***

That style is not supported by Kokkos.

***Cannot use chosen neighbor list style with coul/wolf/kk***

That style is not supported by Kokkos.

***Cannot use chosen neighbor list style with lj/charmm/coul/charmm/implicit/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/charmm/coul/charmm/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/charmm/coul/long/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/class2/coul/cut/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/class2/coul/long/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/class2/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/cut/coul/cut/kk***

That style is not supported by Kokkos.

***Cannot use chosen neighbor list style with lj/cut/coul/debye/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/cut/coul/long/kk***

That style is not supported by Kokkos.

***Cannot use chosen neighbor list style with lj/cut/kk***

That style is not supported by Kokkos.

***Cannot use chosen neighbor list style with lj/expand/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/gromacs/coul/gromacs/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/gromacs/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with lj/spica/kk***

That style is not supported by Kokkos.

***Cannot use chosen neighbor list style with pair eam/kk***

That style is not supported by Kokkos.

***Cannot use chosen neighbor list style with pair eam/kk/alloy***

Self-explanatory.

***Cannot use chosen neighbor list style with pair eam/kk/fs***

Self-explanatory.

***Cannot use chosen neighbor list style with pair sw/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with tersoff/kk***

Self-explanatory.

***Cannot use chosen neighbor list style with tersoff/zbl/kk***

Self-explanatory.

***Cannot use compute chunk/atom bin z for 2d model***

Self-explanatory.

***Cannot use compute cluster/atom unless atoms have IDs***

Atom IDs are used to identify clusters.

***Cannot use create\_atoms rotate unless single style***

Self-explanatory.

***Cannot use create\_bonds unless atoms have IDs***

This command requires a mapping from global atom IDs to local atoms, but the atoms that have been defined have no IDs.

***Cannot use create\_bonds with non-molecular system***

Self-explanatory.

***Cannot use cwiggle in variable formula between runs***

This is a function of elapsed time.

***Cannot use delete\_atoms bond yes with atom\_style template***

This is because the bonds for that atom style are hardwired in the molecule template.

***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 dump\_modify fileper without % in dump file name***

Self-explanatory.

***Cannot use dump\_modify nfile without % in dump file name***

Self-explanatory.

***Cannot use dynamic group with fix adapt atom***

This is not yet supported.

***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 bond/break with non-molecular systems***

Only systems with bonds that can be changed can be used. Atom\_style template does not qualify.

***Cannot use fix bond/create with non-molecular systems***

Only systems with bonds that can be changed can be used. Atom\_style template does not qualify.

***Cannot use fix bond/swap with non-molecular systems***

Only systems with bonds that can be changed can be used. Atom\_style template does not qualify.

***Cannot use fix box/relax on a 2nd non-periodic dimension***

When specifying an off-diagonal pressure component, the second 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 box/relax with both relaxation and scaling on a tilt factor***

When specifying scaling on a tilt factor component, that component can not also be controlled by the barostat. E.g. if scalexy yes is specified and also keyword tri or xy, this is wrong.

***Cannot use fix box/relax with tilt factor scaling on a 2nd non-periodic dimension***

When specifying scaling on a tilt factor component, the second 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 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 trape on a box with zero tilt***

The trape style alters the current strain.

***Cannot use fix deposit rigid and not molecule***

Self-explanatory.

***Cannot use fix deposit rigid and shake***

These two attributes are conflicting.

***Cannot use fix deposit shake and not molecule***

Self-explanatory.

***Cannot use fix enforce2d with 3d simulation***

Self-explanatory.

***Cannot use fix gcmc in a 2d simulation***

Fix gcmc is set up to run in 3d only. No 2d simulations with fix gcmc are allowed.

***Cannot use fix gcmc shake and not molecule***

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 second 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 scaling when y is non-periodic dimension***

The second dimension in the barostatted tilt factor must be periodic.

***Cannot use fix nvt/npt/nph with xz scaling when z is non-periodic dimension***

The second dimension in the barostatted tilt factor must be periodic.

***Cannot use fix nvt/npt/nph with yz scaling when z is non-periodic dimension***

The second dimension in the barostatted tilt factor must be periodic.

***Cannot use fix pour rigid and not molecule***

Self-explanatory.

***Cannot use fix pour rigid and shake***

These two attributes are conflicting.

***Cannot use fix pour shake and not molecule***

Self-explanatory.

***Cannot use fix pour with triclinic box***

This option 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 rigid npt/nph and fix deform on same component of stress tensor***

This would be changing the same box dimension twice.

***Cannot use fix rigid npt/nph on a non-periodic dimension***

When specifying a diagonal pressure component, the dimension must be periodic.

***Cannot use fix rigid/small npt/nph on a non-periodic dimension***

When specifying a diagonal pressure component, the dimension must be periodic.

***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 tune/kSPACE without a kSPACE style***

Self-explanatory.

***Cannot use fix tune/kSPACE without a pair style***

This fix (tune/kSPACE) can only be used when a pair style has been specified.

***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 fix\_deposit unless atoms have IDs***

Self-explanatory.

***Cannot use fix\_pour unless atoms have IDs***

Self-explanatory.

***Cannot use include command within an if command***

Self-explanatory.

***Cannot use lines with fix srd unless overlap is set***

This is because line segments are connected to each other.

***Cannot use multiple fix wall commands with pair brownian***

Self-explanatory.

***Cannot use multiple fix wall commands with pair lubricate***

Self-explanatory.

***Cannot use multiple fix wall commands with pair lubricate/poly***

Self-explanatory.

***Cannot use multiple fix wall commands with pair lubricateU***

Self-explanatory.

***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 beck/gpu pair style***

Self-explanatory.

***Cannot use newton pair with born/coul/long/gpu pair style***

Self-explanatory.

***Cannot use newton pair with born/coul/wolf/gpu pair style***

Self-explanatory.

***Cannot use newton pair with born/gpu pair style***

Self-explanatory.

***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 colloid/gpu pair style***

Self-explanatory.

***Cannot use newton pair with coul/cut/gpu pair style***

Self-explanatory.

***Cannot use newton pair with coul/debye/gpu pair style***

Self-explanatory.

***Cannot use newton pair with coul/dsf/gpu pair style***

Self-explanatory.

***Cannot use newton pair with coul/long/gpu pair style***

Self-explanatory.

***Cannot use newton pair with dipole/cut/gpu pair style***

Self-explanatory.

***Cannot use newton pair with dipole/sf/gpu pair style***

Self-explanatory.

***Cannot use newton pair with dpd/gpu pair style***

Self-explanatory.



*Cannot use newton pair with dpd/tstat/gpu pair style*

Self-explanatory.

*Cannot use newton pair with eam/alloy/gpu pair style*

Self-explanatory.

*Cannot use newton pair with eam/fs/gpu pair style*

Self-explanatory.

*Cannot use newton pair with eam/gpu pair style*

Self-explanatory.

*Cannot use newton pair with gauss/gpu pair style*

Self-explanatory.

*Cannot use newton pair with gayberne/gpu pair style*

Self-explanatory.

*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/cubic/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/debye/gpu pair style*

Self-explanatory.

*Cannot use newton pair with lj/cut/coul/dsf/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/coul/msm/gpu pair style*

Self-explanatory.

*Cannot use newton pair with lj/cut/gpu pair style*

Self-explanatory.

*Cannot use newton pair with lj/expand/gpu pair style*

Self-explanatory.

*Cannot use newton pair with lj/gromacs/gpu pair style*

Self-explanatory.

*Cannot use newton pair with lj/spica/coul/long/gpu pair style*

Self-explanatory.

*Cannot use newton pair with lj/spica/gpu pair style*

Self-explanatory.

*Cannot use newton pair with lj96/cut/gpu pair style*

Self-explanatory.

***Cannot use newton pair with mie/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 soft/gpu pair style***

Self-explanatory.

***Cannot use newton pair with table/gpu pair style***

Self-explanatory.

***Cannot use newton pair with yukawa/colloid/gpu pair style***

Self-explanatory.

***Cannot use newton pair with yukawa/gpu pair style***

Self-explanatory.

***Cannot use newton pair with zbl/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 non-periodic boundaries with fix ttm***

This fix requires a fully periodic simulation box.

***Cannot use non-periodic 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 non-periodic boundaries with EwaldDisp***

For kspace style ewald/disp, 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 non-periodic 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 non-periodic boundaries with PPPMDisp***

For kspace style pppm/disp, 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 package gpu neigh yes with triclinic box***

This is a current restriction in LAMMPS.

***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 read\_data add before simulation box is defined***

Self-explanatory.

***Cannot use read\_data extra with add flag***

Self-explanatory.

***Cannot use read\_data offset without add flag***

Self-explanatory.

***Cannot use read\_data shift without add flag***

Self-explanatory.

***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 efield in fix efield***

LAMMPS computes the energy itself when the E-field is constant.

***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 bias command without temp keyword***

Self-explanatory.

***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 use write\_restart fileper without % in restart file name***

Self-explanatory.

***Cannot use write\_restart nfile without % in restart file name***

Self-explanatory.

***Cannot wiggle and shear fix wall/gran***

Cannot specify both options at the same time.

***Cannot write to restart file - MPI error: %s***

This error was generated by MPI when reading/writing an MPI-IO restart file.

***Cannot yet use KSpace solver with grid with comm style tiled***

This is current restriction in LAMMPS.

***Cannot yet use comm\_style tiled with multi-mode comm***

Self-explanatory.

***Cannot yet use comm\_style tiled with triclinic box***

Self-explanatory.

***Cannot yet use compute tally with Kokkos***

This feature is not yet supported.

***Cannot yet use fix bond/break with this improper style***

This is a current restriction in LAMMPS.

***Cannot yet use fix bond/create with this improper style***

This is a current restriction in LAMMPS.

***Cannot yet use minimize with Kokkos***

This feature is not yet supported.

***Cannot yet use pair hybrid with Kokkos***

This feature is not yet supported.

***Cannot zero Langevin force of 0 atoms***

The group has zero atoms, so you cannot request its force be zeroed.

***Cannot zero gld force for zero atoms***

There are no atoms currently in the group.

***Cannot zero momentum of no atoms***

Self-explanatory.

***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.  $\text{dim} \neq \text{dim1}$  and  $\text{dim} \neq \text{dim2}$ .

***Chunk/atom compute does not exist for compute angmom/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for compute com/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for compute gyration/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for compute inertia/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for compute msd/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for compute omega/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for compute property/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for compute temp/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for compute torque/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for compute vcm/chunk***

Self-explanatory.

***Chunk/atom compute does not exist for fix ave/chunk***

Self-explanatory.

***Comm tiled invalid index in box drop brick***

Internal error check in comm\_style tiled which should not occur. Contact the developers.

***Comm tiled mis-match in box drop brick***

Internal error check in comm\_style tiled which should not occur. Contact the developers.

***Comm\_modify group != atom\_modify first group***

Self-explanatory.

***Communication cutoff for comm\_style tiled cannot exceed periodic box length***

Self-explanatory.

***Communication cutoff too small for SNAP micro load balancing***

This can happen if you change the neighbor skin after your pair\_style command or if your box dimensions grow during a run. You can set the cutoff explicitly via the comm\_modify cutoff command.

***Compute %s does not allow use of dynamic group***

Dynamic groups have not yet been enabled for this compute.

***Compute for fix pafi does not calculate a local array***

Self-explanatory.

***Compute for fix pafi must have 9 fields per atom***

Self-explanatory.

***Compute ID for compute chunk /atom does not exist***

Self-explanatory.

***Compute ID for compute chunk/atom does not exist***

Self-explanatory.

***Compute gyration ID does not exist for compute gyration/shape***

Self-explanatory. Provide a valid compute ID.

***Compute gyration/shape compute ID does not point to a gyration compute***

Self-explanatory. Provide an ID of a compute gyration command.

***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/chunk 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/time does not exist***

Self-explanatory.

***Compute ID for fix numdiff does not exist***

Self-explanatory.

***Compute ID for fix numdiff/virial does not exist***

Self-explanatory.

***Compute ID for fix store/state does not exist***

Self-explanatory.

***Compute ID for fix vector 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 angmom/chunk does not use chunk/atom compute***

The style of the specified compute is not chunk/atom.

***Compute body/local requires atom style body***

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 chunk/atom bin/cylinder radius is too large for periodic box***

Radius cannot be bigger than 1/2 of a non-axis periodic dimension.

***Compute chunk/atom bin/sphere radius is too large for periodic box***

Radius cannot be bigger than 1/2 of any periodic dimension.

***Compute chunk/atom compute array is accessed out-of-range***

The index for the array is out of bounds.

***Compute chunk/atom compute does not calculate a per-atom array***

Self-explanatory.

***Compute chunk/atom compute does not calculate a per-atom vector***

Self-explanatory.

***Compute chunk/atom compute does not calculate per-atom values***

Self-explanatory.

***Compute chunk/atom cylinder axis must be z for 2d***

Self-explanatory.

***Compute chunk/atom fix array is accessed out-of-range***

The index for the array is out of bounds.

***Compute chunk/atom fix does not calculate a per-atom array***

Self-explanatory.

***Compute chunk/atom fix does not calculate a per-atom vector***

Self-explanatory.

***Compute chunk/atom fix does not calculate per-atom values***

Self-explanatory.

***Compute chunk/atom for triclinic boxes requires units reduced***

Self-explanatory.

***Compute chunk/atom ids once but nchunk is not once***

You cannot assign chunks IDs to atom permanently if the number of chunks may change.

***Compute chunk/atom molecule for non-molecular system***

Self-explanatory.

***Compute chunk/atom sphere z origin must be 0.0 for 2d***

Self-explanatory.

***Compute chunk/atom stores no IDs for compute property/chunk***

It will only store IDs if its compress option is enabled.

***Compute chunk/atom stores no coord1 for compute property/chunk***

Only certain binning options for compute chunk/atom store coordinates.

***Compute chunk/atom stores no coord2 for compute property/chunk***

Only certain binning options for compute chunk/atom store coordinates.

***Compute chunk/atom stores no coord3 for compute property/chunk***

Only certain binning options for compute chunk/atom store coordinates.

***Compute chunk/atom variable is not atom-style variable***

Self-explanatory.

***Compute chunk/atom without bins cannot use discard mixed***

That discard option only applies to the binning styles.

***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/chunk does not use chunk/atom compute***

The style of the specified compute is not chunk/atom.

***Compute contact/atom requires a pair style be defined***

Self-explanatory.

***Compute contact/atom requires atom style sphere***

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 dilatation/atom cannot be used with this pair style***

Self-explanatory.

***Compute dilatation/atom requires Peridynamic pair style***

Self-explanatory.

***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 particles.

***Compute erotate/rigid with non-rigid fix-ID***

Self-explanatory.

***Compute erotate/sphere requires atom style sphere***

Self-explanatory.

***Compute erotate/sphere/atom 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/chunk does not use chunk/atom compute***

The style of the specified compute is not chunk/atom.

***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 hexorder/atom cutoff is longer than pairwise cutoff***

Cannot compute order parameter beyond cutoff.

***Compute hexorder/atom requires a pair style be defined***

Self-explanatory.

***Compute improper/local used when impropers are not allowed***

The atom style does not support impropers.

***Compute inertia/chunk does not use chunk/atom compute***

The style of the specified compute is not chunk/atom.

***Compute ke/rigid with non-rigid fix-ID***

Self-explanatory.

***Compute msd/chunk does not use chunk/atom compute***

The style of the specified compute is not chunk/atom.

***Compute msd/chunk nchunk is not static***

This is required because the MSD cannot be computed consistently if the number of chunks is changing. Compute chunk/atom allows setting nchunk to be static.

***Compute nve/asphere requires atom style ellipsoid***

Self-explanatory.

***Compute nvt/nph/npt asphere requires atom style ellipsoid***

Self-explanatory.

***Compute nvt/nph/npt body requires atom style body***

Self-explanatory.

***Compute omega/chunk does not use chunk/atom compute***

The style of the specified compute is not chunk/atom.

***Compute orientorder/atom cutoff is longer than pairwise cutoff***

Cannot compute order parameter beyond cutoff.

***Compute orientorder/atom requires a pair style be defined***

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 plasticity/atom cannot be used with this pair style***

Self-explanatory.

***Compute plasticity/atom requires Peridynamic pair style***

Self-explanatory.

***Compute pressure must use group all***

Virial contributions computed by potentials (pair, bond, etc) are computed on all atoms.

***Compute pressure requires temperature ID to include kinetic energy***

The keflag cannot be used unless a temperature compute is provided.

***Compute pressure temperature ID does not compute temperature***

The compute ID assigned to a pressure computation must compute temperature.

***Compute property/atom floating point vector does not exist***

The command is accessing a vector added by the fix property/atom command, that does not exist.

***Compute property/atom for atom property that is not allocated***

Self-explanatory.

***Compute property/atom integer vector does not exist***

The command is accessing a vector added by the fix property/atom command, that does not exist.

***Compute property/chunk does not use chunk/atom compute***

The style of the specified compute is not chunk/atom.

***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 does not (yet) work with atom\_style template***

Self-explanatory.

***Compute property/local for property that is not allocated***

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 sna/atom cutoff is longer than pairwise cutoff*

Self-explanatory.

*Compute sna/atom requires a pair style be defined*

Self-explanatory.

*Compute snad/atom cutoff is longer than pairwise cutoff*

Self-explanatory.

*Compute snad/atom requires a pair style be defined*

Self-explanatory.

*Compute snav/atom cutoff is longer than pairwise cutoff*

Self-explanatory.

*Compute snav/atom requires a pair style be defined*

Self-explanatory.

*Compute stress/atom temperature ID does not compute temperature*

The specified compute must compute temperature.

*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/body requires atom style body*

Self-explanatory.

*Compute temp/body requires bodies*

This compute can only be applied to body particles.

*Compute temp/chunk does not use chunk/atom compute*

The style of the specified compute is not chunk/atom.

*Compute temp/cs requires ghost atoms store velocity*

Use the comm\_modify vel yes command to enable this.

*Compute temp/cs used when bonds are not allowed*

This compute only works on pairs of bonded particles.

*Compute temp/partial cannot use vz for 2d systemx*

Self-explanatory.

*Compute temp/profile cannot bin z for 2d systems*

Self-explanatory.

*Compute temp/profile cannot use vz for 2d systemx*

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 torque/chunk does not use chunk/atom compute***

The style of the specified compute is not chunk/atom.

***Compute used in dump between runs is not current***

The compute was not invoked on the current timestep, therefore it cannot be used in a dump between runs.

***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 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 page for the variable command for more info.

***Compute vcm/chunk does not use chunk/atom compute***

The style of the specified compute is not chunk/atom.

***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.

***Core/shell partner atom not found***

Could not find one of the atoms in the bond pair.

***Core/shell partners were not all found***

Could not find or more atoms in the bond pairs.

***Could not adjust g\_ewald\_6***

The Newton-Raphson solver failed to converge to a good value for g\_ewald. This error should not occur for typical problems. Please send an email to the developers.

***Could not compute g\_ewald***

The Newton-Raphson solver failed to converge to a good value for g\_ewald. This error should not occur for typical problems. Please send an email to the developers.

***Could not compute grid size***

The code is unable to compute a grid size consistent with the desired accuracy. This error should not occur for typical problems. Please send an email to the developers.

***Could not compute grid size for Coulomb interaction***

The code is unable to compute a grid size consistent with the desired accuracy. This error should not occur for typical problems. Please send an email to the developers.

***Could not compute grid size for Dispersion***

The code is unable to compute a grid size consistent with the desired accuracy. This error should not occur for typical problems. Please send an email to the developers.

***Could not create 3d FFT plan***

The FFT setup for the PPPM solver failed, typically due to lack of memory. This is an unusual error. Check the size of the FFT grid you are requesting.

***Could not create 3d grid of processors***

The specified constraints did not allow a  $P_x$  by  $P_y$  by  $P_z$  grid to be created where  $P_x * P_y * P_z = P$  = total number of processors.

***Could not create 3d remap plan***

The FFT setup in pppm failed.

***Could not create Python function arguments***

This is an internal Python error, possibly because the number of inputs to the function is too large.

***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 evaluate Python function input variable***

Self-explanatory.

***Could not find Python function***

The provided Python code was run successfully, but it not define a callable function with the required name.

***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 msd/chunk fix ID***

The compute creates an internal fix, which has been deleted.

***Could not find compute pressure temperature ID***

The compute ID for calculating temperature does not exist.

***Could not find compute stress/atom temperature ID***

Self-explanatory.

***Could not find compute vacf fix ID***

Self-explanatory.

***Could not find compute/voronoi surface group ID***

Self-explanatory.

***Could not find compute\_modify ID***

Self-explanatory.

***Could not find custom per-atom property 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***

Self-explanatory.

***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 custom atom floating point property ID***

Self-explanatory.

***Could not find dump modify custom atom integer property 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 adapt storage fix ID***

This should not happen unless you explicitly deleted a secondary fix that fix adapt created internally.

***Could not find fix halt variable name***

Self-explanatory.

***Could not find fix gcmc exclusion group ID***

Self-explanatory.

***Could not find fix gcmc rotation group ID***

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 clear group ID***

Self-explanatory.

***Could not find group delete group ID***

Self-explanatory.

***Could not find pair fix ID***

A fix is created internally by the pair style to store shear history information. You cannot delete it.

***Could not find set group ID***

Group ID specified in set command does not exist.

***Could not find specified fix gcmc group ID***

Self-explanatory.

***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.

***Could not initialize embedded Python***

The main module in Python was not accessible.

***Could not open Python file***

The specified file of Python code cannot be opened. Check that the path and name are correct.

***Could not process Python file***

The Python code in the specified file was not run successfully by Python, probably due to errors in the Python code.

***Could not process Python string***

The Python code in the here string was not run successfully by Python, probably due to errors in the Python code.

***Coulomb PPPMDisp order has been reduced below minorder***

The default minimum order is 2. This can be reset by the kspace\_modify minorder command.

***Coulombic cutoff not supported in pair\_style buck/long/coul/coul***

Must use long-range Coulombic interactions.

***Coulombic cutoff not supported in pair\_style lj/long/coul/long***

Must use long-range Coulombic interactions.

***Coulombic cutoff not supported in pair\_style lj/long/tip4p/long***

Must use long-range Coulombic interactions.

***Coulombic cutoffs of pair hybrid sub-styles do not match***

If using a Kspace solver, all Coulombic cutoffs of long pair styles must be the same.

***Coulombic cut not supported in pair\_style lj/long/dipole/long***

Must use long-range Coulombic interactions.

***Cound 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 molecule has atom IDs, but system does not***

The atom\_style id command can be used to force atom IDs to be stored.

***Create\_atoms molecule must have atom types***

The defined molecule does not specify atom types.

***Create\_atoms molecule must have coordinates***

The defined molecule does not specify coordinates.

***Create\_atoms region ID does not exist***

A region ID used in the create\_atoms command does not exist.

***Create\_bonds command before simulation box is defined***

Self-explanatory.

***Create\_bonds command requires no kspace\_style be defined***

This is so that atom pairs that are already bonded to not appear in the neighbor list.

***Create\_bonds command requires special\_bonds 1-2 weights be 0.0***

This is so that atom pairs that are already bonded to not appear in the neighbor list.

***Create\_bonds max distance > neighbor cutoff***

Can only create bonds for atom pairs that will be in neighbor list.

***Create\_bonds requires a pair style be defined***

Self-explanatory.

***Create\_box region ID does not exist***

Self-explanatory.

***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.

***Custom floating point vector for fix store/state does not exist***

The command is accessing a vector added by the fix property/atom command, that does not exist.

***Custom integer vector for fix store/state does not exist***

The command is accessing a vector added by the fix property/atom command, that does not exist.

***Custom per-atom property ID is not floating point***

Self-explanatory.

***Custom per-atom property ID is not integer***

Self-explanatory.

***Cut-offs missing in pair\_style lj/long/dipole/long***

Self-explanatory.

***Cutoffs missing in pair\_style buck/long/coul/long***

Self-explanatory.

***Cutoffs missing in pair\_style lj/long/coul/long***

Self-explanatory.

***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 > max neighbor cutoff***

Can only delete atoms in atom pairs that will be in neighbor list.

***Delete\_atoms mol yes requires atom attribute molecule***

Cannot use this option with a non-molecular system.

***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 assign all restart atoms correctly***

Atoms read in from the restart file were not assigned correctly to processors. This is likely due to some atom coordinates being outside a non-periodic simulation box. Normally this should not happen. You may wish to use the “remap” option on the read\_restart command to see if this helps.

***Did not find all elements in MEAM library file***

Some requested elements were not found in the MEAM file. Check spelling etc.

***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 pressure for fix rigid/nph***

The press keyword must be specified.

***Did not set temp for fix rigid/nvt/small***

Self-explanatory.

***Did not set temp or press for fix rigid/npt/small***

Self-explanatory.

***Did not set temperature for fix rigid/nvt***

The temp keyword must be specified.

***Did not set temperature or pressure for fix rigid/npt***

The temp and press keywords must be specified.

***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 atoms 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/improper extent > half of periodic box length***

This error was detected by the neigh\_modify check yes setting. It is an error because the dihedral atoms are so far apart it is ambiguous how it should be defined.

***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 divedrals allowed***

The chosen atom style does not allow for divedrals to be defined.

***Dihedral\_style command when no divedrals allowed***

The chosen atom style does not allow for divedrals 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 divedrals 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.

***Disk limit not supported by OS or illegal path***

Self-explanatory.

***Dispersion PPPMDisp order has been reduced below minorder***

The default minimum order is 2. This can be reset by the kspace\_modify minorder 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***

This should not normally occur. It is likely a problem with your model.

***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 atom/gz only writes compressed files***

The dump atom/gz output file name must have a .gz suffix.

***Dump cfg arguments can not mix xs|ys|zs with xsu|ysu|zsu***

Self-explanatory.

***Dump cfg arguments must start with 'mass type xs ys zs' or 'mass type xsu ysu zsu'***

This is a requirement of the CFG output format. See the dump cfg doc page for more details.

***Dump cfg requires one snapshot per file***

Use the wildcard "\*" character in the filename.

***Dump cfg/gz only writes compressed files***

The dump cfg/gz output file name must have a .gz suffix.

***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 custom/gz only writes compressed files***

The dump custom/gz output file name must have a .gz suffix.

***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 MPI-IO output not allowed with % in filename***

This is because a % signifies one file per processor and MPI-IO creates one large file for all processors.

***Dump file does not contain requested snapshot***

Self-explanatory.

***Dump file is incorrectly formatted***

Self-explanatory.

***Dump image body yes requires atom style body***

Self-explanatory.

***Dump image bond not allowed with no bond types***

Self-explanatory.

***Dump image cannot perform sorting***

Self-explanatory.

***Dump image line requires atom style line***

Self-explanatory.

***Dump image requires one snapshot per file***

Use a "\*" in the filename.

***Dump image tri requires atom style tri***

Self-explanatory.

***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 xyz/gz only writes compressed files***

The dump xyz/gz output file name must have a .gz suffix.

***Dump\_modify buffer yes not allowed for this style***

Self-explanatory.

***Dump\_modify format string is too short***

There are more fields to be dumped in a line of output than your format string specifies.

***Dump\_modify region ID does not exist***

Self-explanatory.

***Dumping an atom property that is not allocated***

The chosen atom style does not define the per-atom quantity being dumped.

***Duplicate atom IDs exist***

Self-explanatory.

***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.

***Element not defined in potential file***

The specified element is not in the potential file.

***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 did not on this timestep. See the variable page for ideas on how to make this work.

***Epsilon or sigma reference not set by pair style in PPPMDisp***

Self-explanatory.

***Epsilon or sigma reference not set by pair style in ewald/n***

The pair style is not providing the needed epsilon or sigma values.

***Error in MEAM parameter file: keyword %s (further information)***

Self-explanatory. Check the parameter file.

***Error in vdw spline: inner radius > outer radius***

A pre-tabulated spline is invalid. Likely a problem with the potential parameters.

***Error writing averaged chunk data***

Something in the output to the file triggered an error.

***Error writing file header***

Something in the output to the file triggered an error.

***Error writing out correlation data***

Something in the output to the file triggered an error.

***Error writing out histogram data***

Something in the output to the file triggered an error.



**Error writing out time averaged data**

Something in the output to the file triggered an error.

**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 open FFmpeg pipeline to file %s**

The specified file cannot be opened. Check that the path and name are correct and writable and that the FFmpeg executable can be found and run.

**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.

**File variable could not read value**

Check the file assigned to the variable.

**Final box dimension due to fix deform is < 0.0**

Self-explanatory.

**Fix %s does not allow use of dynamic group**

Dynamic groups have not yet been enabled for this fix.

**Fix ID for compute chunk/atom does not exist**

Self-explanatory.

**Fix ID for compute erotate/rigid does not exist**

Self-explanatory.

**Fix ID for compute ke/rigid 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/chunk 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/time does not exist**

Self-explanatory.

**Fix ID for fix store/state does not exist**

Self-explanatory

**Fix ID for fix vector does not exist**

Self-explanatory.

**Fix ID for read\_data does not exist**

Self-explanatory.

***Fix ID for velocity does not exist***

Self-explanatory.

***Fix ID must be alphanumeric or underscore characters***

Self-explanatory.

***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 interface to this pair style not supported***

New coding for the pair style would need to be done.

***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 charge***

The atom style being used does not specify an atom charge.

***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 append/atoms requires a lattice be defined***

Use the lattice command for this purpose.

***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 variable is not atom-style variable***

A variable used by fix ave/atom must generate per-atom values.

***Fix ave/chunk compute does not calculate a per-atom array***

Self-explanatory.

***Fix ave/chunk compute does not calculate a per-atom vector***

Self-explanatory.

***Fix ave/chunk compute does not calculate per-atom values***

Self-explanatory.

***Fix ave/chunk compute vector is accessed out-of-range***

Self-explanatory.

***Fix ave/chunk does not use chunk/atom compute***

The specified compute is not for a compute chunk/atom command.

***Fix ave/chunk fix does not calculate a per-atom array***

Self-explanatory.

***Fix ave/chunk fix does not calculate a per-atom vector***

Self-explanatory.

***Fix ave/chunk fix does not calculate per-atom values***

Self-explanatory.

***Fix ave/chunk fix vector is accessed out-of-range***

Self-explanatory.

***Fix ave/chunk variable is not atom-style variable***

Self-explanatory.

***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 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/weight value and weight vector lengths do not match***

Self-explanatory.

***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 cannot be variable length***

Self-explanatory.

***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 cannot be variable length***

Self-explanatory.

***Fix ave/time fix vector is accessed out-of-range***

The index for the vector is out of bounds.

***Fix ave/time variable is not equal-style variable***

Self-explanatory.

***Fix balance rcb cannot be used with comm\_style brick***

Comm\_style tiled must be used instead.

***Fix balance shift string is invalid***

The string can only contain the characters “x”, “y”, or “z”.

***Fix bond/break needs ghost atoms from further away***

This is because the fix needs to walk bonds to a certain distance to acquire needed info, The comm\_modify cutoff command can be used to extend the communication range.

***Fix bond/create angle type is invalid***

Self-explanatory.

***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 dihedral type is invalid***

Self-explanatory.

***Fix bond/create improper type is invalid***

Self-explanatory.

***Fix bond/create induced too many angles/dihedrals/impropers per atom***

See the read\_data command for info on using the “extra/angle/per/atom”, (or dihedral, improper) keywords to allow for additional angles, dihedrals, and impropers to be formed.

***Fix bond/create needs ghost atoms from further away***

This is because the fix needs to walk bonds to a certain distance to acquire needed info, The comm\_modify cutoff command can be used to extend the communication range.

***Fix bond/react: Cannot use fix bond/react with non-molecular systems***

Only systems with bonds that can be changed can be used. Atom\_style template does not qualify.

***Fix bond/react: Invalid template atom ID in map file***

Atom IDs in molecule templates range from 1 to the number of atoms in the template.

***Fix bond/react: Rmax cutoff is longer than pairwise cutoff***

This is not allowed because bond creation is done using the pairwise neighbor list.

***Fix bond/react: Molecule template ID for fix bond/react does not exist***

A valid molecule template must have been created with the molecule command.

***Fix bond/react: Reaction templates must contain the same number of atoms***

There should be a one-to-one correspondence between atoms in the pre-reacted and post-reacted templates, as specified by the map file.

***Fix bond/react: Unknown section in map file***

Please ensure reaction map files are properly formatted.

***Fix bond/react: Atom/Bond type affected by reaction too close to template edge***

This means an atom which changes type or connectivity during the reaction is too close to an ‘edge’ atom defined in the map file. This could cause incorrect assignment of bonds, angle, etc. Generally, this means you must include more atoms in your templates, such that there are at least two atoms between each atom involved in the reaction and an edge atom.

***Fix bond/react: Fix bond/react needs ghost atoms from farther away***

This is because a processor needs to map the entire unreacted molecule template onto simulation atoms it knows about. The comm\_modify cutoff command can be used to extend the communication range.

***Fix bond/react: A deleted atom cannot remain bonded to an atom that is not deleted***

Self-explanatory.

***Fix bond/react: First neighbors of chiral atoms must be of mutually different types***

Self-explanatory.

***Fix bond/react: Chiral atoms must have exactly four first neighbors***

Self-explanatory.

***Fix bond/react: Molecule template 'Coords' section required for chiralIDs keyword***

The coordinates of atoms in the pre-reacted template are used to determine chirality.

***Fix bond/react special bond generation overflow***

The number of special bonds per-atom created by a reaction exceeds the system setting. See the read\_data or create\_box command for how to specify this value.

***Fix bond/react topology/atom exceed system topology/atom***

The number of bonds, angles etc per-atom created by a reaction exceeds the system setting. See the read\_data or create\_box command for how to specify this value.

***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 yz variable with xy***

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 and fix rigid/small not using same molecule template ID***

Self-explanatory.

***Fix deposit and fix shake not using same molecule template ID***

Self-explanatory.

***Fix deposit molecule must have atom types***

The defined molecule does not specify atom types.

***Fix deposit molecule must have coordinates***

The defined molecule does not specify coordinates.

***Fix deposit molecule template ID must be same as atom\_style template ID***

When using atom\_style template, you cannot deposit molecules that are not in that template.

***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 deposit shake fix does not exist***

Self-explanatory.

***Fix efield requires atom attribute q or mu***

The atom style defined does not have this attribute.

***Fix efield with dipoles cannot use atom-style variables***

This option is not supported.

***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/chunk not computed at compatible time***

Fixes generate their values on specific timesteps. Fix ave/chunk 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 for fix vector not computed at compatible time***

Fixes generate their values on specific timesteps. Fix vector 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 gcmc and fix shake not using same molecule template ID***

Self-explanatory.

***Fix gcmc atom has charge, but atom style does not***

Self-explanatory.

***Fix gcmc cannot exchange individual atoms belonging to a molecule***

This is an error since you should not delete only one atom of a molecule. The user has specified atomic (non-molecular) gas exchanges, but an atom belonging to a molecule could be deleted.



***Fix gcmc does not (yet) work with atom\_style template***

Self-explanatory.

***Fix gcmc molecule command requires that atoms have molecule attributes***

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 has charges, but atom style does not***

Self-explanatory.

***Fix gcmc molecule must have atom types***

The defined molecule does not specify atom types.

***Fix gcmc molecule must have coordinates***

The defined molecule does not specify coordinates.

***Fix gcmc molecule template ID must be same as atom\_style template ID***

When using atom\_style template, you cannot insert molecules that are not in that template.

***Fix gcmc put atom outside box***

This should not normally happen. Contact the developers.

***Fix gcmc ran out of available atom IDs***

See the setting for tagint in the src/lmptype.h file.

***Fix gcmc ran out of available molecule IDs***

See the setting for tagint in the src/lmptype.h file.

***Fix gcmc region cannot be dynamic***

Only static regions can be used with fix gcmc.

***Fix gcmc region does not support a bounding box***

Not all regions represent bounded volumes. You cannot use such a region with the fix gcmc command.

***Fix gcmc region extends outside simulation box***

Self-explanatory.

***Fix gcmc shake fix does not exist***

Self-explanatory.

***Fix gld c coefficients must be  $\geq 0$*** 

Self-explanatory.

***Fix gld needs more prony series coefficients***

Self-explanatory.

***Fix gld prony terms must be  $> 0$*** 

Self-explanatory.

***Fix gld series type must be pprony for now***

Self-explanatory.

***Fix gld start temperature must be  $\geq 0$*** 

Self-explanatory.

***Fix gld stop temperature must be  $\geq 0$*** 

Self-explanatory.

***Fix gld tau coefficients must be  $> 0$*** 

Self-explanatory.

***Fix halt variable is not equal-style variable***

Self-explanatory.

***Fix heat group has no atoms***

Self-explanatory.

***Fix heat kinetic energy of an atom went negative***

This will cause the velocity rescaling about to be performed by fix heat to be invalid.

***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 is not yet implemented with kokkos***

This option is not yet available.

***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 gif and respa are not compatible***

Self-explanatory.

***Fix langevin gif cannot have period equal to dt/2***

If the period is equal to dt/2 then division by zero will happen.

***Fix langevin gif should come before fix nve***

Self-explanatory.

***Fix langevin gif with tbias is not yet implemented with kokkos***

This option is not yet available.

***Fix langevin omega is not yet implemented with kokkos***

This option is not yet available.

***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 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  $0 \leq tscale < 1$***

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 numdiff requires an atom map, see atom\_modify***

Self-explanatory. Efficient loop over all atoms for numerical difference requires an atom map.

***Fix numdiff requires consecutive atom IDs***

Self-explanatory. Efficient loop over all atoms for numerical difference requires consecutive atom IDs.

***Fix numdiff/virial must use group all***

Virial contributions computed by this fix are computed on all atoms.

***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/body requires atom style body***

Self-explanatory.

***Fix nve/body requires bodies***

This fix can only be used for particles that are bodies.

***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 dipole 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 body requires bodies***

Self-explanatory.

***Fix nvt/nph/npt sphere requires atom style sphere***

Self-explanatory.

***Fix nvt/npt/nph damping parameters must be > 0.0***

Self-explanatory.

***Fix nvt/npt/nph 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 and fix rigid/small not using same molecule template ID***

Self-explanatory.

***Fix pour and fix shake not using same molecule template ID***

Self-explanatory.

***Fix pour insertion count per timestep is 0***

Self-explanatory.

***Fix pour molecule must have atom types***

The defined molecule does not specify atom types.

***Fix pour molecule must have coordinates***

The defined molecule does not specify coordinates.

***Fix pour molecule template ID must be same as atom style template ID***

When using atom\_style template, you cannot pour molecules that are not in that template.

***Fix pour polydisperse fractions do not sum to 1.0***

Self-explanatory.

***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 pour rigid fix does not exist***

Self-explanatory.

***Fix pour shake fix does not exist***

Self-explanatory.

***Fix press/berendsen damping parameters must be > 0.0***

Self-explanatory.

***Fix property/atom cannot specify mol twice***

Self-explanatory.

***Fix property/atom cannot specify q twice***

Self-explanatory.

***Fix property/atom mol when atom\_style already has molecule attribute***

Self-explanatory.

***Fix property/atom q when atom\_style already has charge attribute***

Self-explanatory.

***Fix property/atom vector name already exists***

The name for an integer or floating-point vector must be unique.

***Fix qeq has negative upper Taper radius cutoff***

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 qeq/dynamic group has no atoms***

Self-explanatory.

***Fix qeq/dynamic requires atom attribute q***

Self-explanatory.

***Fix qeq/fire group has no atoms***

Self-explanatory.

***Fix qeq/fire requires atom attribute q***

Self-explanatory.

***Fix qeq/point group has no atoms***

Self-explanatory.

***Fix qeq/point has insufficient QEq matrix size***

Occurs when number of neighbor atoms for an atom increased too much during a run. Increase SAFE\_ZONE and MIN\_CAP in fix\_qeq.h and re-compile.

***Fix qeq/point requires atom attribute q***

Self-explanatory.

***Fix qeq/shielded group has no atoms***

Self-explanatory.

***Fix qeq/shielded has insufficient QEq matrix size***

Occurs when number of neighbor atoms for an atom increased too much during a run. Increase SAFE\_ZONE and MIN\_CAP in fix\_qeq.h and re-compile.

***Fix qeq/shielded requires atom attribute q***

Self-explanatory.

***Fix qeq/slater could not extract params from pair coul/streitz***

This should not happen unless pair coul/streitz has been altered.

***Fix qeq/slater group has no atoms***

Self-explanatory.

***Fix qeq/slater has insufficient QEq matrix size***

Occurs when number of neighbor atoms for an atom increased too much during a run. Increase SAFE\_ZONE and MIN\_CAP in fix\_qeq.h and re-compile.

***Fix qeq/slater requires atom attribute q***

Self-explanatory.

***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***

Self-explanatory.

***Fix rigid atom has non-zero image flag in a non-periodic dimension***

Image flags for non-periodic dimensions should not be set.

***Fix rigid file has no lines***

Self-explanatory.

***Fix rigid langevin period must be > 0.0***

Self-explanatory.

***Fix rigid molecule requires atom attribute molecule***

Self-explanatory.

***Fix rigid npt/nph dilate group ID does not exist***

Self-explanatory.

***Fix rigid npt/nph does not yet allow triclinic box***

This is a current restriction in LAMMPS.

***Fix rigid npt/nph period must be > 0.0***

Self-explanatory.

***Fix rigid npt/small t\_chain should not be less than 1***

Self-explanatory.

***Fix rigid npt/small t\_order must be 3 or 5***

Self-explanatory.

***Fix rigid nvt/npt/nph damping parameters must be > 0.0***

Self-explanatory.

***Fix rigid nvt/small t\_chain should not be less than 1***

Self-explanatory.

***Fix rigid nvt/small t\_iter should not be less than 1***

Self-explanatory.

***Fix rigid nvt/small t\_order must be 3 or 5***

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/npt period must be > 0.0***

Self-explanatory.

***Fix rigid/npt temperature order must be 3 or 5***

Self-explanatory.

***Fix rigid/npt/small period must be > 0.0***

Self-explanatory.

***Fix rigid/nvt period must be > 0.0***

Self-explanatory.

***Fix rigid/nvt temperature order must be 3 or 5***

Self-explanatory.

***Fix rigid/nvt/small period must be > 0.0***

Self-explanatory.

***Fix rigid/small atom has non-zero image flag in a non-periodic dimension***

Image flags for non-periodic dimensions should not be set.

***Fix rigid/small langevin period must be > 0.0***

Self-explanatory.

***Fix rigid/small molecule must have atom types***

The defined molecule does not specify atom types.

***Fix rigid/small molecule must have coordinates***

The defined molecule does not specify coordinates.

***Fix rigid/small npt/nph period must be > 0.0***

Self-explanatory.

***Fix rigid/small nvt/npt/nph damping parameters must be > 0.0***

Self-explanatory.

***Fix rigid/small nvt/npt/nph dilate group ID does not exist***

Self-explanatory.

***Fix rigid/small requires an atom map, see atom\_modify***

Self-explanatory.

***Fix rigid/small requires atom attribute molecule***

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 shake molecule template must have shake info***

The defined molecule does not specify SHAKE information.

***Fix spring couple group ID does not exist***

Self-explanatory.

***Fix srd can only currently be used with comm\_style brick***

This is a current restriction in LAMMPS.

***Fix srd lamda must be  $\geq 0.6$  of SRD grid size***

This is a requirement for accuracy reasons.

***Fix srd no-slip requires atom attribute torque***

This is because the SRD collisions will impart torque to the solute particles.

***Fix srd requires SRD particles all have same mass***

Self-explanatory.

***Fix srd requires ghost atoms store velocity***

Use the comm\_modify 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 is not 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/csld is not compatible with fix rattle or fix shake***

These two commands cannot currently be used together with fix temp/csld.

***Fix temp/csld variable returned negative temperature***

Self-explanatory.



***Fix temp/csvr variable returned negative temperature***

Self-explanatory.

***Fix temp/rescale variable returned negative temperature***

Self-explanatory.

***Fix tfmc displacement length must be > 0***

Self-explanatory.

***Fix tfmc is not compatible with fix shake***

These two commands cannot currently be used together.

***Fix tfmc temperature must be > 0***

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 chunk/atom not computed at compatible time***

The chunk/atom compute cannot query the output of the fix on a timestep it is needed.

***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 vector cannot set output array intensive/extensive from these inputs***

The inputs to the command have conflicting intensive/extensive attributes. You need to use more than one fix vector command.

***Fix vector compute does not calculate a scalar***

Self-explanatory.

***Fix vector compute does not calculate a vector***

Self-explanatory.

***Fix vector compute vector is accessed out-of-range***

Self-explanatory.

***Fix vector fix does not calculate a scalar***

Self-explanatory.

***Fix vector fix does not calculate a vector***

Self-explanatory.

***Fix vector fix vector is accessed out-of-range***

Self-explanatory.

***Fix vector variable is not equal-style variable***

Self-explanatory.

***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 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 can not 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 package does not (yet) work with atom\_style template***

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.

***GPUs are requested but Kokkos has not been compiled for CUDA***

Re-compile Kokkos with CUDA support to use GPUs.

***Ghost velocity forward comm not yet implemented with Kokkos***

This is a current restriction.

***Gmask function in equal-style variable formula***

Gmask is per-atom operation.

***Gravity changed since fix pour was created***

The gravity vector defined by fix gravity must be static.

***Gravity must point in -y to use with fix pour in 2d***

Self-explanatory.

***Gravity must point in -z to use with fix pour in 3d***

Self-explanatory.

***Gmask 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 all cannot be made dynamic***

This operation is not allowed.

***Group command before simulation box is defined***

The group command cannot be used before a read\_data, read\_restart, or create\_box command.

***Group dynamic cannot reference itself***

Self-explanatory.

***Group dynamic parent group cannot be dynamic***

Self-explanatory.

***Group dynamic parent group does not exist***

Self-explanatory.

***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 COMB3 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 Vashishta parameter***

One or more of the coefficients defined in the potential file is invalid.

***Illegal compute voronoi/atom command (occupation and (surface or edges))***

Self-explanatory.

***Illegal coul/streitz parameter***

One or more of the coefficients defined in the potential file is invalid.

***Illegal dump\_modify sfactor value (must be > 0.0)***

Self-explanatory.

***Illegal dump\_modify tfactor value (must be > 0.0)***

Self-explanatory.

***Illegal fix gcmc gas mass <= 0***

The computed mass of the designated gas molecule or atom type was less than or equal to zero.

***Illegal fix tfmc random seed***

Seeds can only be nonzero positive integers.

***Illegal fix wall/piston velocity***

The piston velocity must be positive.

***Illegal integrate style***

Self-explanatory.

***Illegal nb3b/harmonic parameter***

One or more of the coefficients defined in the potential file is invalid.

***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 or unset periodicity in restart***

This error should not normally occur unless the restart file is invalid.

***Illegal range increment value***

The increment must be  $\geq 1$ .

***Illegal simulation box***

The lower bound of the simulation box is greater than the upper bound.

***Illegal size double vector read requested***

This error should not normally occur unless the restart file is invalid.

***Illegal size integer vector read requested***

This error should not normally occur unless the restart file is invalid.

***Illegal size string or corrupt restart***

This error should not normally occur unless the restart file is invalid.

***Imageint setting in lmptype.h is invalid***

Imageint must be as large or larger than smallint.

***Imageint setting in lmptype.h is not compatible***

Format of imageint stored in restart file is not consistent with LAMMPS version you are running. See the settings in src/lmptype.h

***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 atoms 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.

***Incompatible KIM Simulator Model***

The requested KIM Simulator Model was defined for a different MD code and thus is not compatible with LAMMPS.

***Incompatible units for KIM Simulator Model***

The selected unit style is not compatible with the requested KIM Simulator Model.

***Incomplete use of variables in create\_atoms command***

The var and set options must be used together.

***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.

***Inconsistent use of finite-size particles by molecule template molecules***

Not all of the molecules define a radius for their constituent particles.

***Incorrect # of floating-point values in Bodies section of data file***

See page for body style.

***Incorrect # of integer values in Bodies section of data file***

See page for body style.

***Incorrect %s format in data file***

A section of the data file being read by fix property/atom does not have the correct number of values per line.

***Incorrect SNAP parameter file***

The file cannot be parsed correctly, check its internal syntax.

***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 atom format in neb file***

The number of fields per line is not what expected.

***Incorrect bonus data format in data file***

See the read\_data 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 EwaldDisp***

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 boundaries with slab PPPMDisp***

Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with ppm/disp.

***Incorrect conversion in format string***

A format style variable was not using either a %f, a %g, or a %e conversion. Or an immediate variable with format suffix was not using either a %f, a %g or a %e conversion in the format suffix.

***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 of ... section in data file***

Number or type of values per line in the given section of the data file is not consistent with the requirements for this section.

***Incorrect format in COMB potential file***

Incorrect number of words per line in the potential file.

***Incorrect format in COMB3 potential file***

Incorrect number of words per line in the potential file.

***Incorrect format in MEAM library file***

Incorrect number of words per line in the potential file.

***Incorrect format in SNAP coefficient file***

Incorrect number of words per line in the coefficient file.

***Incorrect format in SNAP parameter file***

Incorrect number of words per line in the parameter file.

***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 format in Vashishta potential file***

Incorrect number of words per line in the potential file.

***Incorrect format in coul/streitz potential file***

Incorrect number of words per line in the potential file.

***Incorrect format in nb3b/harmonic potential file***

Incorrect number of words per line in the potential file.

***Incorrect integer value in Bodies section of data file***

See page for body style.

***Incorrect multiplicity arg for dihedral coefficients***

Self-explanatory. Check the input script or data file.

***Incorrect number of elements in potential file***

Self-explanatory.

***Incorrect rigid body format in fix rigid file***

The number of fields per line is not what expected.

***Incorrect rigid body format in fix rigid/small 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 table format check for element types***

Self-explanatory.

***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 white-space***

An end quote must be followed by white-space.

***Insertion region extends outside simulation box***

Self-explanatory.

***Insufficient Jacobi rotations for POEMS body***

Eigensolve for rigid body was not sufficiently accurate.

***Insufficient Jacobi rotations for body nparticle***

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 rigid molecule***

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

***Internal error in atom\_style body***

This error should not occur. Contact the developers.

***Invalid -reorder N value***

Self-explanatory.

***Invalid Angles section in molecule file***

Self-explanatory.

***Invalid Bonds section in molecule file***

Self-explanatory.



***Invalid Boolean syntax in if command***

Self-explanatory.

***Invalid Charges section in molecule file***

Self-explanatory.

***Invalid Coords section in molecule file***

Self-explanatory.

***Invalid Diameters section in molecule file***

Self-explanatory.

***Invalid Dihedrals section in molecule file***

Self-explanatory.

***Invalid Improvers section in molecule file***

Self-explanatory.

***Invalid Kokkos command-line args***

Self-explanatory. See Section 2.7 of the manual for details.

***Invalid LAMMPS restart file***

The file does not appear to be a LAMMPS restart file since it does not contain the correct magic string at the beginning.

***Invalid Masses section in molecule file***

Self-explanatory.

***Invalid molecule ID in molecule file***

Molecule ID must be a non-zero positive integer.

***Invalid Molecules section in molecule file***

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 Special Bond Counts section in molecule file***

Self-explanatory.

***Invalid Types section in molecule file***

Self-explanatory.

***Invalid angle count in molecule file***

Self-explanatory.

***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 in Angles section of molecule file***

Self-explanatory.

***Invalid angle type index for fix shake***

Self-explanatory.

***Invalid args for non-hybrid pair coefficients***

“NULL” is only supported in pair\_coeff calls when using pair hybrid

***Invalid argument to factorial %d***

N must be  $\geq 0$  and  $\leq 167$ , otherwise the factorial result is too large.

***Invalid atom ID in %s section of data file***

An atom in a section of the data file being read by fix property/atom has an invalid atom ID that is  $\leq 0$  or  $>$  the maximum existing atom ID.

***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 Angles section of molecule file***

Self-explanatory.

***Invalid atom ID in Atoms section of data file***

Atom IDs must be positive integers.

***Invalid atom ID in Bodies section of data file***

Atom IDs must be positive integers and within range of defined atoms.

***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 Bonds section of molecule file***

Self-explanatory.

***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 Fragments section of molecule file***

Self-explanatory.

***Invalid atom ID in Improvers 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 ID in dihedrals section of molecule file***

Self-explanatory.

***Invalid atom ID in improvers section of molecule file***

Self-explanatory.

***Invalid atom ID in variable file***

Self-explanatory.

***Invalid atom IDs in neb file***

An ID in the file was not found in the system.

***Invalid atom diameter in molecule file***

Diameters must be  $\geq 0.0$ .

***Invalid atom mass for fix shake***

Mass specified in fix shake command must be  $> 0.0$ .

***Invalid atom mass in molecule file***

Masses must be  $> 0.0$ .

***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 create\_atoms mol command***

The atom types in the defined molecule are added to the value specified in the create\_atoms command, as an offset. The final value for each atom must be between 1 to N, where N is the number of atom types.

***Invalid atom type in fix atom/swap command***

The atom type specified in the atom/swap command does not exist.

***Invalid atom type in fix bond/create command***

Self-explanatory.

***Invalid atom type in fix deposit command***

Self-explanatory.

***Invalid atom type in fix deposit mol command***

The atom types in the defined molecule are added to the value specified in the create\_atoms command, as an offset. The final value for each atom must be between 1 to N, where N is the number of atom types.

***Invalid atom type in fix gcmc command***

The atom type specified in the gcmc command does not exist.

***Invalid atom type in fix pour command***

Self-explanatory.

***Invalid atom type in fix pour mol command***

The atom types in the defined molecule are added to the value specified in the create\_atoms command, as an offset. The final value for each atom must be between 1 to N, where N is the number of atom types.

***Invalid atom type in molecule file***

Atom types must range from 1 to specified # of types.

***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 atom\_style body command***

No body style argument was provided.

***Invalid atom\_style command***

Self-explanatory.

***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 basis setting in create\_atoms command***

The basis index must be between 1 to N where N is the number of basis atoms in the lattice. The type index must be between 1 to N where N is the number of atom types.

***Invalid basis setting in fix append/atoms command***

The basis index must be between 1 to N where N is the number of basis atoms in the lattice. The type index must be between 1 to N where N is the number of atom types.

***Invalid bin bounds in compute chunk/atom***

The lo/hi values are inconsistent.

***Invalid bin bounds in fix ave/spatial***

The lo/hi values are inconsistent.

***Invalid body nparticle command***

Arguments in atom-style command are not correct.

***Invalid bond count in molecule file***

Self-explanatory.

***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 Bonds section of molecule file***

Self-explanatory.

***Invalid bond type in create\_bonds command***

Self-explanatory.

***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 color map min/max values***

The min/max values are not consistent with either each other or with values in the color map.

***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 create\_atoms rotation vector for 2d model***

The rotation vector can only have a z component.

***Invalid custom OpenCL parameter string.***

There are not enough or too many parameters in the custom string for package GPU.

***Invalid cutoff in comm\_modify command***

Specified cutoff must be  $\geq 0.0$ .

***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: Bodies***

Atom style does not allow bodies.

***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  $\leq 0.0$ .

***Invalid density in set command***

Density must be  $> 0.0$ .

***Invalid diameter in set command***

Self-explanatory.

***Invalid dihedral count in molecule file***

Self-explanatory.

***Invalid dihedral type in Dihedrals section of data file***

Dihedral type must be positive integer and within range of specified dihedral types.

***Invalid dihedral type in dihedrals section of molecule file***

Self-explanatory.

***Invalid dipole length in set command***

Self-explanatory.

***Invalid displace\_atoms rotate axis for 2d***

Axis must be in z direction.

***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 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 movie filename***

The file produced by dump movie cannot be binary or compressed and must be a single file for a single processor.

***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 is 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 halt attribute***

Self-explanatory.

***Invalid fix halt operator***

Self-explanatory.

***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 qeq parameter file***

Element index > number of atom types.

***Invalid fix rigid npt/nph command for a 2d simulation***

Cannot control z dimension in a 2d model.

***Invalid fix rigid npt/nph command pressure settings***

If multiple dimensions are coupled, those dimensions must be specified.

***Invalid fix rigid/small npt/nph command for a 2d simulation***

Cannot control z dimension in a 2d model.

***Invalid fix rigid/small npt/nph command pressure settings***

If multiple dimensions are coupled, those dimensions must be specified.

***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 peratom section of restart file***

The format of this section of the file is not correct.

***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 comm\_modify command***

Self-explanatory.

***Invalid image up vector***

Up vector cannot be (0,0,0).

***Invalid immediate variable***

Syntax of immediate value is incorrect.

***Invalid improper count in molecule file***

Self-explanatory.

***Invalid improper type in Improvers section of data file***

Improper type must be positive integer and within range of specified improper types.

***Invalid improper type in improvers section of molecule file***

Self-explanatory.

***Invalid index for non-body particles in compute body/local command***

Only indices 1,2,3 can be used for non-body particles.

***Invalid index in compute body/local command***

Self-explanatory.

***Invalid is\_active() function in variable formula***

Self-explanatory.

***Invalid is\_available() function in variable formula***

Self-explanatory.

***Invalid is\_defined() function in variable formula***

Self-explanatory.

***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/chunk command***

Self-explanatory.

***Invalid keyword in compute property/local 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 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 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 param file for fix qeq/shielded***

Invalid value of gamma.

***Invalid param file for fix qeq/slater***

Zeta value is 0.0.

***Invalid partitions in processors part command***

Valid partitions are numbered 1 to N and the sender and receiver cannot be the same partition.

***Invalid python 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.

***Invalid radius in Atoms section of data file***

Radius must be  $\geq 0.0$ .

***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 replace values in compute reduce***

Self-explanatory.

***Invalid rigid body ID in fix rigid file***

The ID does not match the number of an existing ID of rigid bodies that are defined by the fix rigid command.

***Invalid rigid body ID in fix rigid/small file***

The ID does not match the number of an existing ID of rigid bodies that are defined by the fix rigid/small 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 shake angle type in molecule file***

Self-explanatory.

***Invalid shake atom in molecule file***

Self-explanatory.

***Invalid shake bond type in molecule file***

Self-explanatory.

***Invalid shake flag in molecule file***

Self-explanatory.

***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 atom index in molecule file***

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 template atom in Atoms section of data file***

The atom indices must be between 1 to N, where N is the number of atoms in the template molecule the atom belongs to.

***Invalid template index in Atoms section of data file***

The template indices must be between 1 to N, where N is the number of molecules in the template.

***Invalid thermo keyword in variable formula***

The keyword is not recognized.

***Invalid threads\_per\_atom specified.***

For 3-body potentials on the GPU, the threads\_per\_atom setting cannot be greater than 4 for NVIDIA GPUs.

***Invalid timestep reset for fix ave/atom***

Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

***Invalid timestep reset for fix ave/chunk***

Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

***Invalid timestep reset for fix ave/correlate***

Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

***Invalid timestep reset for fix ave/histo***

Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

***Invalid timestep reset for fix ave/spatial***

Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

***Invalid timestep reset for fix ave/time***

Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

***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 label2type() function syntax in variable formula***

The first argument must be a label map kind (atom, bond, angle, dihedral, or improper) and the second argument must be a valid type label that has been assigned to a numeric type.

***Invalid use of library file() function***

This function is called through the library interface. This error should not occur. Contact the developers if it does.

***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 in special function next***

Only file-style or atomfile-style variables can be used with next().

***Invalid variable style with next command***

Variable styles *equal* and *world* cannot be used in a next command.

***Invalid volume in set command***

Volume must be > 0.0.

***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.

***Invoking coulombic in pair style lj/coul requires atom attribute q***

The atom style defined does not have this attribute.

***Invoking coulombic in pair style lj/long/dipole/long requires atom attribute q***

The atom style defined does not have these attributes.

***KIM Simulator Model has no Model definition***

There is no model definition (key: model-defn) in the KIM Simulator Model. Please contact the OpenKIM database maintainers to verify and potentially correct this.

***KOKKOS package does not yet support comm\_style tiled***

Self-explanatory.

***KOKKOS package requires a kokkos enabled atom\_style***

Self-explanatory.

***KSpace accuracy must be > 0***

The kspace accuracy designated in the input must be greater than zero.

***KSpace accuracy too large to estimate G vector***

Reduce the accuracy request or specify gewald explicitly via the kspace\_modify command.

***KSpace accuracy too low***

Requested accuracy must be less than 1.0.

***KSpace solver requires a pair style***

No pair style is defined.

***KSpace style does not yet support triclinic geometries***

The specified kspace style does not allow for non-orthogonal simulation boxes.

***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 matching long-range Coulombic or dispersion components be used.

***Keyword %s in MEAM parameter file not recognized***

Self-explanatory.

***Kokkos has been compiled for CUDA but no GPUs are requested***

One or more GPUs must be used when Kokkos is compiled for CUDA.

***Kspace\_modify mesh parameter must be all zero or all positive***

Valid kspace mesh parameters are >0. The code will try to auto-detect suitable values when all three mesh sizes are set to zero (the default).

***Kspace\_modify mesh/disp parameter must be all zero or all positive***

Valid kspace mesh/disp parameters are >0. The code will try to auto-detect suitable values when all three mesh sizes are set to zero **and** the required accuracy via *force/disp/real* as well as *force/disp/kspace* is set.

***Kspace style does not support compute group/group***

Self-explanatory.

***Kspace style pppm/disp/tip4p requires newton on***

Self-explanatory.

***Kspace style pppm/tip4p requires newton on***

Self-explanatory.

***Kspace style requires atom attribute q***

The atom style defined does not have these attributes.

***Kspace\_modify eigtol must be smaller than one***

Self-explanatory.

***LAMMPS is not built with Python embedded***

This is done by including the PYTHON package before LAMMPS is built. This is required to use python-style variables.

***LAMMPS unit\_style lj not supported by KIM models***

Self-explanatory. Check the input script or data file.

***LJ6 off not supported in pair\_style buck/long/coul/long***

Self-explanatory.

***Label map is incomplete: all types must be assigned a unique type label***

For a given type-kind (atom types, bond types, etc.) to be written to the data file, all associated types must be assigned a type label, and each type label can be assigned to only one numeric type.

***Label wasn't found in input script***

Self-explanatory.

***Labelmap command before simulation box is defined***

The labelmap command cannot be used before a read\_data, read\_restart, or create\_box command.

***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  $\mathbf{a}_1 \times \mathbf{a}_2 = \mathbf{a}_3$ .

***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 subdomain away before reneighboring.

***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.

***MSM can only currently be used with comm\_style brick***

This is a current restriction in LAMMPS.

***MSM grid is too large***

The global MSM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 16384.

You likely need to decrease the requested accuracy.

***MSM order must be 4, 6, 8, or 10***

This is a limitation of the MSM implementation in LAMMPS: the MSM order can only be 4, 6, 8, or 10.

***Mass command before simulation box is defined***

The mass command cannot be used before a read\_data, read\_restart, or create\_box command.

***Matrix factorization to split dispersion coefficients failed***

This should not normally happen. Contact the developers.

***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 an 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 parameter in MEAM library file: z!=lat***

The coordination number and lattice do not match, check that consistent values are given.

***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.

***Modulo 0 in variable formula***

Self-explanatory.

***Molecule IDs too large for compute chunk/atom***

The IDs must not be larger than can be stored in a 32-bit integer since chunk IDs are 32-bit integers.

***Molecule auto special bond generation overflow***

Counts exceed maxspecial setting for other atoms in system.

***Molecule file has angles but no nangles setting***

Self-explanatory.

***Molecule file has body params but no setting for them***

Self-explanatory.

***Molecule file has bonds but no nbonds setting***

Self-explanatory.

***Molecule file has dihedrals but no ndihedrals setting***

Self-explanatory.

***Molecule file has fragments but no nfragments setting***

Self-explanatory.

***Molecule file has impropers but no nimpropers setting***

Self-explanatory.

***Molecule file has no Body Doubles section***

Self-explanatory.

***Molecule file has no Body Integers section***

Self-explanatory.

***Molecule file has no Fragments section***

Self-explanatory.

***Molecule file has special flags but no bonds***

Self-explanatory.

***Molecule file needs both Special Bond sections***

Self-explanatory.

***Molecule file requires atom style body***

Self-explanatory.

***Molecule file shake flags not before shake atoms***

The order of the two sections is important.

***Molecule file shake flags not before shake bonds***

The order of the two sections is important.

***Molecule file shake info is incomplete***

All 3 SHAKE sections are needed.

***Molecule file special list does not match special count***

The number of values in an atom's special list does not match count.

***Molecule file z center-of-mass must be 0.0 for 2d***

Self-explanatory.

***Molecule file z coord must be 0.0 for 2d***

Self-explanatory.

***Molecule natoms must be 1 for body particle***

Self-explanatory.

***Molecule sizescale must be 1.0 for body particle***

Self-explanatory.

***Molecule template ID for atom\_style template does not exist***

Self-explanatory.

***Molecule template ID for create\_atoms does not exist***

Self-explanatory.

***Molecule template ID for fix deposit does not exist***

Self-explanatory.

***Molecule template ID for fix gcmc does not exist***

Self-explanatory.

***Molecule template ID for fix pour does not exist***

Self-explanatory.

***Molecule template ID for fix rigid/small does not exist***

Self-explanatory.

***Molecule template ID for fix shake does not exist***

Self-explanatory.

***Molecule template ID must be alphanumeric or underscore characters***

Self-explanatory.

***Molecule topology/atom exceeds system topology/atom***

The number of bonds, angles, etc per-atom in the molecule exceeds the system setting. See the create\_box command for how to specify these values.

***Molecule topology type exceeds system topology type***

The number of bond, angle, etc types in the molecule exceeds the system setting. See the create\_box command for how to specify these values.

***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.

***Mu not allowed when not using semi-grand in fix atom/swap command***

Self-explanatory.

***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 pair\_style before Pair Coeffs***

Must use a pair\_style command before reading a data file that defines Pair Coeffs.

***Must define pair\_style before PairIJ Coeffs***

Must use a pair\_style command before reading a data file that defines PairIJ 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 not have multiple fixes change box parameter ...***

Self-explanatory.

***Must read Angle Type Labels before Angles***

An Angle Type Labels section of a data file must come before the Angles section.

***Must read Atom Type Labels before Atoms***

An Atom Type Labels section of a data file must come before the Atoms section.

***Must read Atoms before Angles***

The Atoms section of a data file must come before an Angles section.

***Must read Atoms before Bodies***

The Atoms section of a data file must come before a Bodies 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 Improvers***

The Atoms section of a data file must come before an Improvers 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 read Bond Type Labels before Bonds***

A Bond Type Labels section of a data file must come before the Bonds section.

***Must read Dihedral Type Labels before Dihedrals***

An Dihedral Type Labels section of a data file must come before the Dihedrals section.

***Must read Improper Type Labels before Improvers***

An Improper Type Labels section of a data file must come before the Improvers section.

***Must re-specify non-restarted pair style (xxx) after read\_restart***

For pair styles, that do not store their settings in a restart file, it must be defined with a new 'pair\_style' command after read\_restart.

***Must set both respa inner and outer***

Cannot use just the inner or outer option with respa without using the other.

***Must set number of threads via package omp command***

Because you are using the OPENMP package, set the number of threads via its settings, not by the pair\_style snap nthreads setting.

***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***

Self-explanatory.

***Must specify at least 2 types in fix atom/swap command***

Self-explanatory.

***Must use 'kim\_style init' command before simulation box is defined***

Self-explanatory.

***Must use 'kim\_style define' command after simulation box is defined***

Self-explanatory.

***Must use 'kim\_style init' command before 'kim\_style define'***

Self-explanatory.

***Must use 'kspace\_modify pressure/scalar no' for rRESPA with kspace\_style MSM***

The kspace scalar pressure option cannot (yet) be used with rRESPA.

***Must use 'kspace\_modify pressure/scalar no' for tensor components with kspace\_style msm***

Otherwise MSM will compute only a scalar pressure. See the kspace\_modify command for details on this setting.

***Must use 'kspace\_modify pressure/scalar no' to obtain per-atom virial with kspace\_style MSM***

The kspace scalar pressure option cannot be used to obtain per-atom virial.

***Must use 'kspace\_modify pressure/scalar no' with GPU MSM Pair styles***

The kspace scalar pressure option is not (yet) compatible with GPU MSM Pair styles.

***Must use 'kspace\_modify pressure/scalar no' with kspace\_style msm/cg***

The kspace scalar pressure option is not compatible with kspace\_style msm/cg.

***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 Kokkos half/thread or full neighbor list with threads or GPUs***

Using Kokkos half-neighbor lists with threading is not allowed.

***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 region with fix pour***

Self-explanatory.

***Must use an angle style with TIP4P potential***

TIP4P potentials assume angles in water are constrained by a fix shake command.

***Must use atom map style array with Kokkos***

See the atom\_modify map command.

***Must use atom style with molecule IDs with fix bond/swap***

Self-explanatory.

***Must use pair\_style comb or comb3 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.

***Must use variable energy with fix efield***

You must define an energy when performing a minimization with a variable E-field.

***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.

***Need nswaptypes mu values in fix atom/swap command***

Self-explanatory.

***Needed bonus data not in data file***

Some atom styles require bonus data. See the read\_data page for details.

***Needed molecular topology not in data file***

The header of the data file indicated bonds, angles, etc would be included, but they are 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 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 atom IDs exceed maximum allowed ID***

See the setting for tagint in the src/lmptype.h file.

***New bond exceeded bonds per atom in create\_bonds***

See the read\_data command for info on using the “extra/bond/per/atom” keyword to allow for additional bonds to be formed

***New bond exceeded bonds per atom in fix bond/create***

See the read\_data command for info on using the “extra/bond/per/atom” keyword to allow for additional bonds to be formed

***New bond exceeded special list size in fix bond/create***

See the “read\_data extra/special/per/atom” command (or the “create\_box extra/special/per/atom” 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.

***Next command must list all universe and uloop variables***

This is to ensure they stay in sync.

***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***

Self-explanatory.

***No atoms in data file***

The header of the data file indicated that atoms would be included, but they are not present.

***No basis atoms in lattice***

Basis atoms must be defined for lattice style user.

***No bodies allowed with this atom style***

Self-explanatory. Check data file.

***No bond style is defined for compute bond/local***

Self-explanatory.

***No bonds allowed with this atom style***

Self-explanatory.

***No box information in dump. You have to use 'box no'***

Self-explanatory.

***No count or invalid atom count in molecule file***

The number of atoms must be specified.

***No dihedral style is defined for compute dihedral/local***

Self-explanatory.

***No dihedrals allowed with this atom style***

Self-explanatory.

***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***

Self-explanatory. Check data file.

***No fix gravity defined for fix pour***

Gravity is required to use fix pour.

***No improper style is defined for compute improper/local***

Self-explanatory.

***No impropers allowed with this atom style***

Self-explanatory.

***No input values for fix ave/spatial***

Self-explanatory.

***No lines allowed with this atom style***

Self-explanatory. Check data file.

***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 molecule topology allowed with atom style template***

The data file cannot specify the number of bonds, angles, etc, because this info is inferred from the molecule templates.

***No overlap of box and region for create\_atoms***

Self-explanatory.

***No pair coul/streitz for fix qeq/slater***

These commands must be used together.

***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***

Self-explanatory. Check data file.

***No values in fix ave/chunk command***

Self-explanatory.

***No values in fix ave/time command***

Self-explanatory.

***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.

***Non-numeric box dimensions - simulation unstable***

The box size has apparently blown up.

***Non-zero atom IDs with atom\_modify id = no***

Self-explanatory.

***Non-zero read\_data shift z value for 2d simulation***

Self-explanatory.

***Nprocs not a multiple of N for -reorder***

Self-explanatory.

***Number of core atoms != number of shell atoms***

There must be a one-to-one pairing of core and shell atoms.

***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 Atom IDs is negative***

Atom IDs must be positive integers.

***One or more atom IDs is too big***

The limit on atom IDs is set by the SMALLBIG, BIGBIG, SMALLSMALL setting in your LAMMPS build. See the [Build settings](#) page for more info.

***One or more atom IDs is zero***

Either all atoms IDs must be zero or none of them.

***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 more rigid bodies are a single particle***

Self-explanatory.

***One or zero atoms in rigid body***

Any rigid body defined by the fix rigid command must contain 2 or more atoms.

***Only 2 types allowed when not using semi-grand in fix atom/swap command***

Self-explanatory.

***Only one cut-off allowed when requesting all long***

Self-explanatory.

***Only one cutoff allowed when requesting all long***

Self-explanatory.

***Only zhi currently implemented for fix append/atoms***

Self-explanatory.

***Out of range atoms - cannot compute MSM***

One or more atoms are attempting to map their charge to a MSM 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 subdomain 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 subdomain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

***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 subdomain 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 subdomain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

***Out of range atoms - cannot compute PPPMDisp***

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 subdomain 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 subdomain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

***Overflow of allocated fix vector storage***

This should not normally happen if the fix correctly calculated how long the vector will grow to. Contact the developers.

***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 can only currently be used with comm\_style brick***

This is a current restriction in LAMMPS.

***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 grid stencil extends beyond nearest neighbor processor***

This is not allowed if the kspace\_modify overlap setting is no.

***PPPM order < minimum allowed order***

The default minimum order is 2. This can be reset by the kspace\_modify minorder command.

***PPPM order cannot be < 2 or > than %d***

This is a limitation of the PPPM implementation in LAMMPS.

***PPPMDisp Coulomb 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.

***PPPMDisp Dispersion 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.

***PPPMDisp can only currently be used with comm\_style brick***

This is a current restriction in LAMMPS.

***PPPMDisp coulomb order cannot be greater than %d***

This is a limitation of the PPPM implementation in LAMMPS.

***PPPMDisp used but no parameters set, for further information please see the ppm/disp documentation***

An efficient and accurate usage of the ppm/disp requires settings via the kspace\_modify command. Please see the ppm/disp documentation for further instructions.

***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.

***Package command after simulation box is defined***

The package command cannot be used after a read\_data, read\_restart, or create\_box command.

***Package gpu command without GPU package installed***

The GPU package must be installed via “make yes-gpu” before LAMMPS is built.

***Package intel command without INTEL package installed***

The INTEL package must be installed via “make yes-intel” before LAMMPS is built.

***Package kokkos command without KOKKOS package enabled***

The KOKKOS package must be installed via “make yes-kokkos” before LAMMPS is built, and the “-k on” must be used to enable the package.

***Package omp command without OPENMP package installed***

The OPENMP package must be installed via “make yes-openmp” before LAMMPS is built.

***Pair body requires atom style body***

Self-explanatory.



***Pair body requires body style nparticle***

This pair style is specific to the nparticle body style.

***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 dipole/cut/gpu requires atom attributes q, mu, torque***

The atom style defined does not have this attribute.

***Pair dipole/long requires atom attributes q, mu, torque***

The atom style defined does not have these attributes.

***Pair dipole/sf/gpu requires atom attributes q, mu, torque***

The atom style defined does not one or more of 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 comm\_modify 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 attributes radius, rmass***

The atom style defined does not have these attributes.

***Pair granular requires ghost atoms store velocity***

Use the comm\_modify 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 single calls do not support per sub-style special bond values***

Self-explanatory.

***Pair hybrid sub-style does not support single call***

You are attempting to invoke a single() call on a pair style that does not 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 lj/long/dipole/long requires atom attributes mu, torque***

The atom style defined does not have these attributes.

***Pair lubricate requires atom style sphere***

Self-explanatory.

***Pair lubricate requires ghost atoms store velocity***

Use the comm\_modify 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 comm\_modify 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 comm\_modify 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 comm\_modify 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 COMB3 requires atom IDs***

This is a requirement to use the COMB3 potential.

***Pair style COMB3 requires atom attribute q***

Self-explanatory.

***Pair style COMB3 requires newton pair on***

See the newton command. This is a restriction to use the COMB3 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 Tersoff potential.

***Pair style MEAM requires newton pair on***

See the newton command. This is a restriction to use the MEAM potential.

***Pair style SNAP requires newton pair on***

See the newton command. This is a restriction to use the SNAP 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 Vashishta requires atom IDs***

This is a requirement to use the Vashishta potential.

***Pair style Vashishta requires newton pair on***

See the newton command. This is a restriction to use the Vashishta 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 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/long/gpu requires atom attribute q***

The atom style defined does not have this attribute.

***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 buck/long/coul/long 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/cut/gpu requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style coul/debye/gpu requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style coul/dsf requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style coul/dsf/gpu requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style coul/long/gpu requires atom attribute q***

The atom style defined does not have these attributes.

***Pair style coul/streitz requires atom attribute q***

Self-explanatory.

***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 can not 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 can not 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 can not 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 can not be invoked by fix bond/swap.

***Pair style does not support pair\_write***

The pair style does not have a single() function, so it can not 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***

Self-explanatory.

***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 is incompatible with TIP4P KSpace style***

The pair style does not have the requires TIP4P settings.

***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/debye/gpu requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style lj/cut/coul/dsf requires atom attribute q***

The atom style defined does not have these attributes.

***Pair style lj/cut/coul/dsf/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/tip4p/cut requires atom IDs***

This is a requirement to use this potential.

***Pair style lj/cut/tip4p/cut requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style lj/cut/tip4p/cut requires newton pair on***

See the newton command. This is a restriction to use this potential.

***Pair style lj/cut/tip4p/long 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/tip4p/long requires atom attribute q***

The atom style defined does not have these attributes.

***Pair style lj/cut/tip4p/long 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 lj/long/dipole/long does not currently support respa***

This feature is not yet supported.

***Pair style lj/long/tip4p/long 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/long/tip4p/long requires atom attribute q***

The atom style defined does not have these attributes.

***Pair style lj/long/tip4p/long 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/spica/coul/long/gpu requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style nb3b/harmonic requires atom IDs***

This is a requirement to use this potential.

***Pair style nb3b/harmonic requires newton pair on***

See the newton command. This is a restriction to use this potential.

***Pair style nm/cut/coul/cut requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style nm/cut/coul/long requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style peri requires atom style peri***

Self-explanatory.

***Pair style polymorphic requires atom IDs***

This is a requirement to use the polymorphic potential.

***Pair style polymorphic requires newton pair on***

See the newton command. This is a restriction to use the polymorphic potential.

***Pair style reax requires atom IDs***

This is a requirement to use the ReaxFF potential.

***Pair style reax requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style reax requires newton pair on***

This is a requirement to use the ReaxFF potential.

***Pair style requires a KSpace style***

No kspace style is defined.

***Pair style requires use of kspace\_style ewald/disp***

Self-explanatory.

***Pair style sw/gpu requires atom IDs***

This is a requirement to use this potential.

***Pair style sw/gpu requires newton pair off***

See the newton command. This is a restriction to use this potential.

***Pair style vashishta/gpu requires atom IDs***

This is a requirement to use this potential.

***Pair style vashishta/gpu requires newton pair off***

See the newton command. This is a restriction to use this potential.

***Pair style tersoff/gpu requires atom IDs***

This is a requirement to use the tersoff/gpu potential.

***Pair style tersoff/gpu requires newton pair off***

See the newton command. This is a restriction to use this pair style.

***Pair style tip4p/cut requires atom IDs***

This is a requirement to use this potential.

***Pair style tip4p/cut requires atom attribute q***

The atom style defined does not have this attribute.

***Pair style tip4p/cut requires newton pair on***

See the newton command. This is a restriction to use this potential.

***Pair style tip4p/long 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 tip4p/long requires atom attribute q***

The atom style defined does not have these attributes.

***Pair style tip4p/long 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 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 tersoff/zbl/kk 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 yukawa/colloid/gpu requires atom style sphere***

Self-explanatory.

***PairKIM only works with 3D problems***

This is a current limitation.

***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\_modify special setting for pair hybrid incompatible with global special\_bonds setting***

Cannot override a setting of 0.0 or 1.0 or change a setting between 0.0 and 1.0.



***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 outside surface of region used in fix wall/region***

Particles must be inside the region for energy/force to be calculated. A particle outside the region generates an error.

***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 did not on this timestep. See the variable 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 did not on this timestep. See the variable 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 has more than one entry for the same element.

***Potential file is missing an entry***

The potential file 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 fix rigid npt/nph does not exist***

Self-explanatory.

***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/body***

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/body***

Self-explanatory.

***Pressure control must be used with fix nph/small***

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/body***

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 do not match number of allocated processors***

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 vales 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.

***Python function evaluation failed***

The Python function did not run successfully and/or did not return a value (if it is supposed to return a value). This is probably due to some error condition in the function.

***Python function is not callable***

The provided Python code was run successfully, but it not define a callable function with the required name.

***Python invoke of undefined function***

Cannot invoke a function that has not been previously defined.

***Python variable does not match Python function***

This matching is defined by the python-style variable and the python command.

***Python variable has no function***

No python command was used to define the function associated with the python-style variable.

***QEQ with 'newton pair off' not supported***

See the newton command. This is a restriction to use the QEQ fixes.

***R0 < 0 for fix spring command***

Equilibrium spring length is invalid.

***RATTLE coordinate constraints are not satisfied up to desired tolerance***

Self-explanatory.

***RATTLE determinant = 0.0***

The determinant of the matrix being solved for a single cluster specified by the fix rattle command is numerically invalid.

***RATTLE failed***

Certain constraints were not satisfied.

***RATTLE velocity constraints are not satisfied up to desired tolerance***

Self-explanatory.

***Read data add offset is too big***

It cannot be larger than the size of atom IDs, e.g. the maximum 32-bit integer.

***Read dump of atom property that is not allocated***

Self-explanatory.

***Read rerun dump file timestep > specified stop***

Self-explanatory.

***Read restart MPI-IO input not allowed with % in filename***

This is because a % signifies one file per processor and MPI-IO creates one large file for all processors.

***Read\_data shrink wrap did not assign all atoms correctly***

This is typically because the box-size specified in the data file is large compared to the actual extent of atoms in a shrink-wrapped dimension. When LAMMPS shrink-wraps the box atoms will be lost if the processor they are re-assigned to is too far away. Choose a box size closer to the actual extent of the atoms.

***Read\_dump command before simulation box is defined***

The read\_dump command cannot be used before a read\_data, read\_restart, or create\_box command.

***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 xyz fields do not have consistent scaling/wrapping***

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 chunk/atom does not exist***

Self-explanatory.

***Region ID for compute reduce/region does not exist***

Self-explanatory.

***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 atom/swap 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 efield does not exist***

Self-explanatory.

***Region ID for fix evaporate does not exist***

Self-explanatory.

***Region ID for fix gcmc 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 for group dynamic 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 for fix oneway does not exist***

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 second time, but only if the style matches the previous fix. In this case it is assumed you want 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 system atom IDs are too big***

See the setting for tagint in the src/lmptype.h file.

***Replicated system is too big***

See the setting for bigint in the src/lmptype.h file.

***Required border comm not yet implemented with Kokkos***

There are various limitations in the communication options supported by Kokkos.

***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 size 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  $\leq$  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 file MPI-IO output not allowed with % in filename***

This is because a % signifies one file per processor and MPI-IO creates one large file for all processors.

***Restart file byte ordering is not recognized***

The file does not appear to be a LAMMPS restart file since it does not contain a recognized byte-ordering flag at the beginning.

***Restart file byte ordering is swapped***

The file was written on a machine with different byte-ordering than the machine you are reading it on. Convert it to a text data file instead, on the machine you wrote it on.

***Restart file incompatible with current version***

This is probably because you are trying to read a file created with a version of LAMMPS that is too old compared to the current version. Use your older version of LAMMPS and convert the restart file to a data file.

***Restart file is a MPI-IO file***

The file is inconsistent with the filename you specified for it.

***Restart file is a multi-proc file***

The file is inconsistent with the filename you specified for it.

***Restart file is not a MPI-IO file***

The file is inconsistent with the filename you specified for it.

***Restart file is not a multi-proc file***

The file is inconsistent with the filename you specified for it.

***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 three 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 two 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 molecule template ID***

The template IDs must be unique.

***Reuse of region ID***

A region ID cannot be used twice.

***Rigid body atoms %d %d missing on proc %d at step %ld***

This means that an atom cannot find the atom that owns the rigid body it is part of, or vice versa. The solution is to use the communicate cutoff command to ensure ghost atoms are acquired from far enough away to encompass the max distance printed when the fix rigid/small command was invoked.

***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.

***SRD particle %d started inside wall %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 floating point vector does not exist***

Self-explanatory.

***Set command integer vector does not exist***

Self-explanatory.

***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 two 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 three 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 two 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.

***Shear history 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.

***Small to big integers are not sized correctly***

This error occurs when the sizes of smallint, imageint, tagint, bigint, as defined in src/lmptype.h are not what is expected. Contact the developers if this occurs.

***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.

***Special list size exceeded in fix bond/create***

See the “read\_data extra/special/per/atom” command (or the “create\_box extra/special/per/atom” command) for info on how to leave space in the special bonds list to allow for additional bonds to be formed.

***Species XXX is not supported by this KIM Simulator Model***

The kim\_style define command was referencing a species that is not present in the requested KIM Simulator Model.

***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.

***Subsequent read data induced too many angles per atom***

See the extra/angle/per/atom keyword for the create\_box or the read\_data command to set this limit larger

***Subsequent read data induced too many bonds per atom***

See the extra/bond/per/atom keyword for the create\_box or the read\_data command to set this limit larger

***Subsequent read data induced too many dihedrals per atom***

See the extra/dihedral/per/atom keyword for the create\_box or the read\_data command to set this limit larger

***Subsequent read data induced too many improper per atom***

See the extra/improper/per/atom keyword for the create\_box or the read\_data command to set this limit larger

***Substitution for illegal variable***

Input script line contained a variable that could not be substituted for.



***Support for writing images in JPEG format not included***

LAMMPS was not built with the -DLAMMPS\_JPEG switch in the Makefile.

***Support for writing images in PNG format not included***

LAMMPS was not built with the -DLAMMPS\_PNG switch in the Makefile.

***Support for writing movies not included***

LAMMPS was not built with the -DLAMMPS\_FFMPEG switch in the Makefile

***System in data file is too big***

See the setting for bigint in the src/lmptype.h file.

***System is not charge neutral, net charge = %g***

The total charge on all atoms on the system is not 0.0. For some KSpace solvers this is an error.

***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***

Self-explanatory.

***Tagint setting in lmptype.h is invalid***

Tagint must be as large or larger than smallint.

***Tagint setting in lmptype.h is not compatible***

Format of tagint stored in restart file is not consistent with LAMMPS version you are running. See the settings in src/lmptype.h

***Target pressure for fix rigid/nph cannot be < 0.0***

Self-explanatory.

***Target pressure for fix rigid/npt/small cannot be < 0.0***

Self-explanatory.

***Target temperature for fix nvt/npt/nph cannot be 0.0***

Self-explanatory.

***Target temperature for fix rigid/npt cannot be 0.0***

Self-explanatory.

***Target temperature for fix rigid/npt/small cannot be 0.0***

Self-explanatory.

***Target temperature for fix rigid/nvt cannot be 0.0***

Self-explanatory.

***Target temperature for fix rigid/nvt/small 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/npt does not exist***

Self-explanatory.

***Temperature ID for fix press/berendsen does not exist***

Self-explanatory.

***Temperature ID for fix rigid nvt/npt/nph does not exist***

Self-explanatory.

***Temperature ID for fix temp/berendsen does not exist***

Self-explanatory.

***Temperature ID for fix temp/csld does not exist***

Self-explanatory.

***Temperature ID for fix temp/csvr does not exist***

Self-explanatory.

***Temperature ID for fix temp/rescale does not exist***

Self-explanatory.

***Temperature compute degrees of freedom < 0***

This should not happen if you are calculating the temperature on a valid set of atoms.

***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/body***

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/body***

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/body***

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 control must not be used with fix nph/small***

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).

***Test\_descriptor\_string already allocated***

This is an internal error. Contact the developers.

***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 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 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 every variable returned a bad timestep***

The returned timestep is less than or equal to the current timestep.

***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 is not 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 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 few lines in %s section of data file***

Self-explanatory.

***Too few values in body lines in data file***

Self-explanatory.

***Too few values in body section of molecule file***

Self-explanatory.

***Too many -pk arguments in command line***

The string formed by concatenating the arguments is too long. Use a package command in the input script instead.

***Too many MSM grid levels***

The max number of MSM grid levels is hardwired to 10.

***Too many args in variable function***

More args are used than any variable function allows.

***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 elements extracted from MEAM library.***

Increase 'maxelt' in meam.h and recompile.

***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 lines in one body in data file - boost MAXBODY***

MAXBODY is a setting at the top of the src/read\_data.cpp file. Set it larger and re-compile the code.

***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 molecules for fix poems***

The limit is  $2^{31} = \sim 2$  billion molecules.

***Too many molecules for fix rigid***

The limit is  $2^{31} = \sim 2$  billion molecules.

***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 values in body lines in data file***

Self-explanatory.

***Too many values in body section of molecule file***

Self-explanatory.

***Too much buffered per-proc info for dump***

The size of the buffered string must fit in a 32-bit integer for a dump.

***Too much per-proc info for dump***

Number of local atoms times number of columns must fit in a 32-bit integer for dump.

***Topology type exceeds system topology type***

The number of bond, angle, etc types exceeds the system setting. See the create\_box or read\_data command for how to specify these values.

***Tree structure in joint connections***

Fix poems cannot (yet) work with coupled bodies whose joints connect the bodies in a tree structure.

***Tried to convert a double to int, but input\_double > INT\_MAX***

Self-explanatory.

***Trying to build an occasional neighbor list before initialization completed***

This is not allowed. Source code caller needs to be modified.

***Two fix ave commands using same compute chunk/atom command in incompatible ways***

They are both attempting to “lock” the chunk/atom command so that the chunk assignments persist for some number of timesteps, but are doing it in different ways.

***Two groups cannot be the same in fix spring couple***

Self-explanatory.

***The %s type label %s is already in use for type %s***

For a given type-kind (atom types, bond types, etc.), a given type label can be assigned to only one numeric type.

***Type label string %s for %s type %s is invalid***

See the labelmap command documentation for valid type labels.

***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 empty line in Angle Coeffs section***

Read a blank line where there should be coefficient data.

***Unexpected empty line in Bond Coeffs section***

Read a blank line where there should be coefficient data.

***Unexpected empty line in Dihedral Coeffs section***

Read a blank line where there should be coefficient data.

***Unexpected empty line in Improper Coeffs section***

Read a blank line where there should be coefficient data.

***Unexpected empty line in Pair Coeffs section***

Read a blank line where there should be coefficient data.

***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.

***Unexpected end of fix rigid/small file***

A read operation from the file failed.

***Unexpected end of molecule file***

Self-explanatory.

***Unexpected end of neb 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  $\geq$  to the number of processor partitions.

***Unrecognized angle style***

The choice of angle style is unknown.

***Unrecognized atom style***

The choice of atom style is unknown.

***Unrecognized body style***

The choice of body style is unknown.

***Unrecognized bond style***

The choice of bond style is unknown.

***Unknown category for info is\_active()***

Self-explanatory.

***Unknown category for info is\_available()***

Self-explanatory.

***Unknown category for info is\_defined()***

Self-explanatory.

***Unrecognized command: %s***

The command is not known to LAMMPS. Check the input script.

***Unrecognized compute style***

The choice of compute style is unknown.

***Unrecognized dihedral style***

The choice of dihedral style is unknown.

***Unrecognized dump reader style***

The choice of dump reader style via the format keyword is unknown.

***Unrecognized dump style***

The choice of dump style is unknown.

***Unknown error in GPU library***

Self-explanatory.

***Unrecognized fix style***

The choice of fix style is unknown.

***Unknown identifier in data file: %s***

A section of the data file cannot be read by LAMMPS.

***Unrecognized improper style***

The choice of improper style is unknown.

***Unknown keyword in thermo\_style custom command***

One or more specified keywords are not recognized.

***Unrecognized kspace style***

The choice of kspace style is unknown.

***Unknown name for info newton category***

Self-explanatory.

***Unknown name for info package category***

Self-explanatory.

***Unknown name for info pair category***

Self-explanatory.

***Unrecognized pair style***

The choice of pair style is unknown.

***Unknown pair\_modify hybrid sub-style***

The choice of sub-style is unknown.

***Unrecognized region style***

The choice of region style is unknown.

***Unknown section in molecule file***

Self-explanatory.

***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.

***Unknown unit\_style***

Self-explanatory. Check the input script or data file.



***Unrecognized lattice type in MEAM library file***

The lattice type in an entry of the MEAM library file is not valid.

***Unrecognized lattice type in MEAM parameter file***

The lattice type in an entry of the MEAM parameter file is not valid.

***Unrecognized pair style in compute pair command***

Self-explanatory.

***Unsupported mixing rule in kspace\_style ewald/disp***

Only geometric mixing is supported.

***Unsupported order in kspace\_style ewald/disp***

Only  $1/r^6$  dispersion or dipole terms are supported.

***Unsupported order in kspace\_style ppm/disp, pair\_style %s***

Only pair styles with  $1/r$  and  $1/r^6$  dependence are currently supported.

***Unsupported parameter in MEAM library file***

Self-explanatory.

***Use cutoff keyword to set cutoff in single mode***

Mode is single so cutoff/multi keyword cannot be used.

***Use cutoff/multi keyword to set cutoff in multi mode***

Mode is multi so cutoff keyword cannot be used.

***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.

***Using suffix gpu without GPU package installed***

Self-explanatory.

***Using suffix intel without INTEL package installed***

Self-explanatory.

***Using suffix kk without KOKKOS package enabled***

Self-explanatory.

***Using suffix omp without OPENMP package installed***

Self-explanatory.

***Using update dipole flag requires atom attribute mu***

Self-explanatory.

***Using update dipole flag requires atom style sphere***

Self-explanatory.

***Variable ID in variable formula does not exist***

Self-explanatory.

***Variable atom ID is too large***

Specified ID is larger than the maximum allowed atom ID.

***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 evaluation in fix wall gave bad value***

The returned value for epsilon or sigma < 0.0.

***Variable evaluation in region gave bad value***

Variable returned a radius < 0.0.

***Variable for compute ti is invalid style***

Self-explanatory.

***Variable for create\_atoms is invalid style***

The variables must be equal-style variables.

***Variable for displace\_atoms is invalid style***

It must be an equal-style or atom-style variable.

***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 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***

The variable must be an equal- or atom-style variable.

***Variable for fix gravity is invalid style***

Only equal-style variables can be used.

***Variable for fix heat is invalid style***

Only equal-style or atom-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/csld is invalid style***

Only equal-style variables can be used.

***Variable for fix temp/csvr 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 group dynamic is invalid style***

The variable must be an atom-style variable.

***Variable for group is invalid style***

Only atom-style variables can be used.

***Variable for region cylinder is invalid style***

Only equal-style variables are allowed.

***Variable for region is invalid style***

Only equal-style variables can be used.

***Variable for region is not equal style***

Self-explanatory.

***Variable for region sphere is invalid style***

Only equal-style variables are allowed.

***Variable for restart is invalid style***

Only equal-style variables can be used.

***Variable for set command is invalid style***

Only atom-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 for voronoi radius is not atom style***

Self-explanatory.

*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 has circular dependency*

A circular dependency is when variable “a” is used by variable “b” and variable “b” is also used by variable “a”. Circular dependencies with longer chains of dependence are also not allowed.

*Variable name between brackets must be alphanumeric or underscore characters*

Self-explanatory.

*Variable name for compute chunk/atom 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 create\_atoms does not exist*

Self-explanatory.

*Variable name for displace\_atoms 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 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/chunk 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*

Self-explanatory.

*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 heat 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/csld does not exist*

Self-explanatory.

*Variable name for fix temp/csvr does not exist*

Self-explanatory.

*Variable name for fix temp/rescale does not exist*

Self-explanatory.

*Variable name for fix vector 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 group does not exist***

Self-explanatory.

***Variable name for group dynamic does not exist***

Self-explanatory.

***Variable name for region cylinder does not exist***

Self-explanatory.

***Variable name for region does not exist***

Self-explanatory.

***Variable name for region sphere does not exist***

Self-explanatory.

***Variable name for restart does not exist***

Self-explanatory.

***Variable name for set command 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 for voronoi radius does not exist***

Self-explanatory.

***Variable name must be alphanumeric or underscore characters***

Self-explanatory.

***Variable uses atom property that is not allocated***

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 rigid used with non-rigid fix-ID***

Self-explanatory.

***Velocity temperature ID does calculate a velocity bias***

The specified compute must compute a bias for temperature.

***Velocity temperature ID does not compute temperature***

The compute ID given to the velocity command must compute temperature.

***Verlet/split can only currently be used with comm\_style brick***

This is a current restriction in LAMMPS.

***Verlet/split does not yet support TIP4P***

This is a current limitation.

***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 did not on this timestep. See the variable page for ideas on how to make this work.

***Voro++ error: narea and neigh have a different size***

This error is returned by the Voro++ library.

***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/tip4p/cut***

This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

***Water H epsilon must be 0.0 for pair style lj/cut/tip4p/long***

This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

***Water H epsilon must be 0.0 for pair style lj/long/tip4p/long***

This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

***World variable count does not match # of partitions***

A world-style variable must specify a number of values equal to the number of processor partitions.

***Write\_data command before simulation box is defined***

Self-explanatory.

***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 rotation vector with displace\_atoms***

Self-explanatory.

***Zero length rotation vector with fix move***

Self-explanatory.

***Zero-length lattice orient vector***

Self-explanatory.

## 11.6 Warning messages

This is an alphabetic list of the WARNING messages LAMMPS prints out and the reason why. If the explanation here is not sufficient, the documentation for the offending command may help. Warning messages also list the source file and line number where the warning was generated. For example, a message like this:

WARNING: Bond atom missing in box size check (domain.cpp:187)

means that line #187 in the file src/domain.cpp generated the error. Looking in the source code may help you figure out what went wrong.

Doc page with [ERROR messages](#)

---

***Adjusting Coulombic cutoff for MSM, new cutoff = %g***

The adjust/cutoff command is turned on and the Coulombic cutoff has been adjusted to match the user-specified accuracy.

***Angle atoms missing at step %ld***

One or more of three 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 style in data file differs from currently defined angle style***

Self-explanatory.

***Angles are defined but no angle style is set***

The topology contains angles, but there are no angle forces computed since there was no angle\_style command.

***Atom style in data file differs from currently defined atom style***

Self-explanatory.

***Bond atom missing in box size check***

The second atom 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 image check***

The second atom in 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 atoms missing at step %ld***

The second atom 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 style in data file differs from currently defined bond style***

Self-explanatory.

***Bonds are defined but no bond style is set***

The topology contains bonds, but there are no bond forces computed since there was no bond\_style command.

***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.

***Both groups in compute group/group have a net charge; the Kspace boundary correction to energy will be non-zero***

Self-explanatory.



***Calling write\_dump before a full system init.***

The write\_dump command is used before the system has been fully initialized as part of a ‘run’ or ‘minimize’ command. Not all dump styles and features are fully supported at this point and thus the command may fail or produce incomplete or incorrect output. Insert a “run 0” command, if a full system init is required.

***Cannot count rigid body degrees-of-freedom before bodies are fully initialized***

This means the temperature associated with the rigid bodies may be incorrect on this timestep.

***Cannot count rigid body degrees-of-freedom before bodies are initialized***

This means the temperature associated with the rigid bodies may be incorrect on this timestep.

***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.

***Charges are set, but coulombic solver is not used***

Self-explanatory.

***Charges did not converge at step %ld: %lg***

Self-explanatory.

***Communication cutoff is 0.0. No ghost atoms will be generated. Atoms may get lost***

The communication cutoff defaults to the maximum of what is inferred from pair and bond styles (will be zero, if none are defined) and what is specified via [comm\\_modify cutoff](#) (defaults to 0.0). If this results to 0.0, no ghost atoms will be generated and LAMMPS may lose atoms or use incorrect periodic images of atoms in interaction lists. To avoid, either use [pair style zero](#) with a suitable cutoff or use [comm\\_modify cutoff](#).

***Communication cutoff is shorter than a bond length based estimate. This may lead to errors.***

Since LAMMPS stores topology data with individual atoms, all atoms comprising a bond, angle, dihedral or improper must be present on any subdomain that “owns” the atom with the information, either as a local or a ghost atom. The communication cutoff is what determines up to what distance from a subdomain boundary ghost atoms are created. The communication cutoff is by default the largest non-bonded cutoff plus the neighbor skin distance, but for short or non-bonded cutoffs and/or long bonds, this may not be sufficient. This warning indicates that there is an increased risk of a simulation stopping unexpectedly because of Bond/Angle/Dihedral/Improper atoms missing. It can be silenced by manually setting the communication cutoff via [comm\\_modify cutoff](#). However, since the heuristic used to determine the estimate is not always accurate, it is not changed automatically and the warning may be ignored depending on the specific system being simulated.

***Communication cutoff is too small for SNAP micro load balancing, increased to %lf***

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.

***Create\_bonds max distance > minimum neighbor cutoff***

This means atom pairs for some atom types may not be in the neighbor list and thus no bond can be created between them.

***Delete\_atoms cutoff > minimum neighbor cutoff***

This means atom pairs for some atom types may not be in the neighbor list and thus an atom in that pair cannot be deleted.

***Dihedral atoms missing 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 problem***

Conformation of the 4 listed dihedral atoms is extreme; you may want to check your simulation geometry.

***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.

***Dihedral style in data file differs from currently defined dihedral style***

Self-explanatory.

***Dihedrals are defined but no dihedral style is set***

The topology contains dihedrals, but there are no dihedral forces computed since there was no dihedral\_style command.

***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.

***Energy due to X extra global DOFs will be included in minimizer energies***

When using fixes like box/relax, the potential energy used by the minimizer is augmented by an additional energy provided by the fix. Thus the printed converged energy may be different from the total potential energy.

***Estimated error in splitting of dispersion coeffs is %g***

Error is greater than 0.0001 percent.

***Ewald/disp Newton solver failed, using old method to estimate g\_ewald***

Self-explanatory. Choosing a different cutoff value may help.

***FENE bond too long***

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 %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 halt condition for fix-id %s met on step %ld with value %g***

Self explanatory.

***Fix SRD walls overlap but fix srd overlap not set***

You likely want to set this in your input script.

***Fix bond/create is used multiple times or with fix bond/break - may not work as expected***

When using fix bond/create multiple times or in combination with fix bond/break, the individual fix instances do not share information about changes they made at the same time step and thus it may result in unexpected behavior.

***Fix bond/react: Atom affected by reaction too close to template edge***

This means an atom which changes type or connectivity during the reaction is too close to an 'edge' atom defined in the superimpose file. This could cause incorrect assignment of bonds, angle, etc. Generally, this means you must include more atoms in your templates, such that there are at least two atoms between each atom involved in the reaction and an edge atom.

***Fix bond/swap will ignore defined angles***

See the page for fix bond/swap for more info on this restriction.

***Fix deposit near setting < possible overlap separation %g***

This test is performed for finite size particles with a diameter, not for point particles. The near setting is smaller than the particle diameter which can lead to overlaps.

***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 gcmc using full\_energy option***

Fix gcmc has automatically turned on the full\_energy option since it is required for systems like the one specified by the user. User input included one or more of the following: kspace, triclinic, a hybrid pair style, an eam pair style, or no “single” function for the pair style.

***Fix langevin gif using random gaussians is not implemented with kokkos***

This will most likely cause errors in kinetic fluctuations.

***Fix property/atom mol or charge w/out ghost communication***

A model typically needs these properties defined for ghost atoms.

***Fix qeq CG convergence failed (%g) after %d iterations at %ld step***

Self-explanatory.

***Fix qeq has non-zero lower Taper radius cutoff***

Absolute value must be  $\leq 0.01$ .

***Fix qeq has very low Taper radius cutoff***

Value should typically be  $\geq 5.0$ .

***Fix qeq/dynamic tolerance may be too small for damped dynamics***

Self-explanatory.

***Fix qeq/fire tolerance may be too small for damped fires***

Self-explanatory.

***Fix rattle should come after all other integration fixes***

This fix is designed to work after all other integration fixes change atom positions. Thus it should be the last integration fix specified. If not, it will not satisfy the desired constraints as well as it otherwise would.

***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 srd SRD moves may trigger frequent reneighboring***

This is because the SRD particles may move long distances.

***Fix srd grid size > 1/4 of big particle diameter***

This may cause accuracy problems.

***Fix srd particle moved outside valid domain***

This may indicate a problem with your simulation parameters.

***Fix srd particles may move > big particle diameter***

This may cause accuracy problems.

***Fix srd viscosity < 0.0 due to low SRD density***

This may cause accuracy problems.

***Fixes cannot send data in Kokkos communication, switching to classic communication***

This is current restriction with Kokkos.

***For better accuracy use ‘pair\_modify table 0’***

The user-specified force accuracy cannot be achieved unless the table feature is disabled by using ‘pair\_modify table 0’.

***Geometric mixing assumed for  $1/r^6$  coefficients***

Self-explanatory.

***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.

***H matrix size has been exceeded: m\_fill=%d H.m=%dn***

This is the size of the matrix.

***Ignoring unknown or incorrect info command flag***

Self-explanatory. An unknown argument was given to the info command. Compare your input with the documentation.

***Improper atoms missing 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 problem: %d %ld %d %d %d %d***

Conformation of the 4 listed improper atoms is extreme; you may want to check your simulation geometry.

***Improper style in data file differs from currently defined improper style***

Self-explanatory.

***Impropers are defined but no improper style is set***

The topology contains impropers, but there are no improper forces computed since there was no improper\_style command.

***Inconsistent image flags***

The image flags for a pair on bonded atoms appear to be inconsistent. Inconsistent means that when the coordinates of the two atoms are unwrapped using the image flags, the two atoms are far apart. Specifically they are further apart than half a periodic box length. Or they are more than a box length apart in a non-periodic dimension. This is usually due to the initial data file not having correct image flags for the two atoms in a bond that straddles a periodic boundary. They should be different by 1 in that case. This is a warning because inconsistent image flags will not cause problems for dynamics or most LAMMPS simulations. However they can cause problems when such atoms are used with the fix rigid or replicate commands. Note that if you have an infinite periodic crystal with bonds then it is impossible to have fully consistent image flags, since some bonds will cross periodic boundaries and connect two atoms with the same image flag.

***Increasing communication cutoff for GPU style***

The pair style has increased the communication cutoff to be consistent with the communication cutoff requirements for this pair style when run on the GPU.

***KIM Model does not provide 'energy'; Potential energy will be zero***

Self-explanatory.

***KIM Model does not provide 'forces'; Forces will be zero***

Self-explanatory.

***KIM Model does not provide 'particleEnergy'; energy per atom will be zero***

Self-explanatory.

***KIM Model does not provide 'particleVirial'; virial per atom will be zero***

Self-explanatory.

***Kspace\_modify slab param < 2.0 may cause unphysical behavior***

The kspace\_modify slab parameter should be larger to ensure periodic grids padded with empty space do not overlap.

***Less insertions than requested***

The fix pour command was unsuccessful at finding open space for as many particles as it tried to insert.

***Library error in lammgs\_gather\_atoms***

This library function cannot be used if atom IDs are not defined or are not consecutively numbered.

***Library error in lammmps\_scatter\_atoms***

This library function cannot be used if atom IDs are not defined or are not consecutively numbered, or if no atom map is defined. See the atom\_modify command for details about atom maps.

***Likewise 1-2 special neighbor interactions != 1.0***

The topology contains bonds, but there is no bond style defined and a 1-2 special neighbor scaling factor was not 1.0. This means that pair style interactions may have scaled or missing pairs in the neighbor list in expectation of interactions for those pairs being computed from the bond style.

***Likewise 1-3 special neighbor interactions != 1.0***

The topology contains angles, but there is no angle style defined and a 1-3 special neighbor scaling factor was not 1.0. This means that pair style interactions may have scaled or missing pairs in the neighbor list in expectation of interactions for those pairs being computed from the angle style.

***Likewise 1-4 special neighbor interactions != 1.0***

The topology contains dihedrals, but there is no dihedral style defined and a 1-4 special neighbor scaling factor was not 1.0. This means that pair style interactions may have scaled or missing pairs in the neighbor list in expectation of interactions for those pairs being computed from the dihedral style.

***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 subdomain away before reneighboring.

***MSM mesh too small, increasing to 2 points in each direction***

Self-explanatory.

***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.

***Mixing forced for lj coefficients***

Self-explanatory.

***Molecule attributes do not match system attributes***

An attribute is specified (e.g. diameter, charge) that is not defined for the specified atom style.

***Molecule has bond topology but no special bond settings***

This means the bonded atoms will not be excluded in pairwise interactions.

***Molecule template for create\_atoms has multiple molecules***

The create\_atoms command will only create molecules of a single type, i.e. the first molecule in the template.

***Molecule template for fix gcmc has multiple molecules***

The fix gcmc command will only create molecules of a single type, i.e. the first molecule in the template.

***Molecule template for fix shake has multiple molecules***

The fix shake command will only recognize molecules of a single type, i.e. the first molecule in the template.

***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 contact/atom***

It is not efficient to use compute contact/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 dilatation/atom***

Self-explanatory.

***More than one compute erotate/sphere/atom***

It is not efficient to use compute erotate/sphere/atom more than once.

***More than one compute hexorder/atom***

It is not efficient to use compute hexorder/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 compute orientorder/atom***

It is not efficient to use compute orientorder/atom more than once.

***More than one compute plasticity/atom***

Self-explanatory.

***More than one compute sna/atom***

Self-explanatory.

***More than one compute sna/grid***

Self-explanatory.

***More than one compute sna/grid/local***

Self-explanatory.

***More than one compute snad/atom***

Self-explanatory.

***More than one compute snav/atom***

Self-explanatory.

***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.

***Neighbor exclusions used with KSpace solver may give inconsistent Coulombic energies***

This is because excluding specific pair interactions also excludes them from long-range interactions which may not be the desired effect. The special\_bonds command handles this consistently by ensuring excluded (or weighted) 1-2, 1-3, 1-4 interactions are treated consistently by both the short-range pair style and the long-range solver. This is not done for exclusions of charged atom pairs via the neigh\_modify exclude command.

***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 second partition performs a kspace calculation so the kspace\_style command must be used.

***No automatic unit conversion to XTC file format conventions possible for units lj***

This means no scaling will be performed.

***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 reaxff***

This is most likely an error, unless you have created your own ReaxFF parameter file in a different set of units.

***Number of MSM mesh points changed to be a multiple of 2***

MSM requires that the number of grid points in each direction be a multiple of two and the number of grid points in one or more directions have been adjusted to meet this requirement.

***OMP\_NUM\_THREADS environment is not set.***

This environment variable must be set appropriately to use the OPENMP package.

***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 chunks do not contain all atoms in molecule***

This may not be what you intended.

***One or more dynamic groups may not be updated at correct point in timestep***

If there are other fixes that act immediately after the initial stage of time integration within a timestep (i.e. after atoms move), then the command that sets up the dynamic group should appear after those fixes. This will ensure that dynamic group assignments are made after all atoms have moved.

***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.

***Pair style in data file differs from currently defined pair style***

Self-explanatory.

***Pair style restartinfo set but has no restart support***

This pair style has a bug, where it does not support reading and writing information to a restart file, but does not set the member variable "restartinfo" to 0 as required in that case.

***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.

***Proc subdomain size < neighbor skin, could lead to lost atoms***

The decomposition of the physical domain (likely due to load balancing) has led to a processor's subdomain being smaller than the neighbor skin in one or more dimensions. Since reneighboring is triggered by atoms moving the skin distance, this may lead to lost atoms, if an atom moves all the way across a neighboring processor's subdomain before reneighboring is triggered.

***Reducing PPPM order b/c stencil extends beyond nearest neighbor processor***

This may lead to a larger grid than desired. See the kspace\_modify overlap command to prevent changing of the PPPM order.

***Reducing PPPMDisp Coulomb order b/c stencil extends beyond neighbor processor***

This may lead to a larger grid than desired. See the kspace\_modify overlap command to prevent changing of the PPPM order.

***Reducing PPPMDisp dispersion order b/c stencil extends beyond neighbor processor***

This may lead to a larger grid than desired. See the kspace\_modify overlap command to prevent changing of the PPPM order.

***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.



***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 lamda***

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.

***SRD particle %d started inside wall %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.

***Shell command '%s' failed with error '%s'***

Self-explanatory.

***Shell command returned with non-zero status***

This may indicate the shell command did not operate as expected.

***Should not allow rigid bodies to bounce off reflecting walls***

LAMMPS allows this, but their dynamics are not computed correctly.

***Should not use fix nve/limit with fix shake or fix rattle***

This will lead to invalid constraint forces in the SHAKE/RATTLE computation.

***Simulations might be very slow because of large number of structure factors***

Self-explanatory.

***Slab correction not needed for MSM***

Slab correction is intended to be used with Ewald or PPPM and is not needed by MSM.

***Specifying an 'subset' value of '0' is equivalent to no 'subset' keyword***

Self-explanatory.

***System is not charge neutral, net charge = %g***

The total charge on all atoms on the system is not 0.0. For some KSpace solvers this is only a warning.

***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.

***The fix ave/spatial command has been replaced by the more flexible fix ave/chunk and compute chunk/atom commands – fix ave/spatial will be removed in the summer of 2015***

Self-explanatory.

***The minimizer does not re-orient dipoles when using fix efield***

This means that only the atom coordinates will be minimized, not the orientation of the dipoles.

***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 a many-body potential with bonds/angles/dihedrals and special\_bond exclusions***

This is likely not what you want to do. The exclusion settings will eliminate neighbors in the neighbor list, which the many-body potential needs to calculate its terms correctly.

***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 kspace solver on system with no charge***

Self-explanatory.

***Using largest cut-off for lj/long/dipole/long long long***

Self-explanatory.

***Using largest cutoff for buck/long/coul/long***

Self-explanatory.

***Using largest cutoff for lj/long/coul/long***

Self-explanatory.

***Using largest cutoff for pair\_style lj/long/tip4p/long***

Self-explanatory.

***Using package gpu without any pair style defined***

Self-explanatory.

***Using pair potential shift with pair\_modify compute no***

The shift effects will thus not be computed.

***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.

***Using pair tail corrections with pair\_modify compute no***

The tail corrections will thus not be computed.