LAMMPS Developer's Guide

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This document is a developer's guide to the LAMMPS molecular dynamics package, whose WWW site is at lammps.sandia.gov. It describes the internal structure and algorithms of the code. Sections will be added as we have time, and in response to requests from developers and users.

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1 LAMMPS source files

LAMMPS source files are in two directories of the distribution tarball. The src directory has the majority of them, all of which are C++ files (*.cpp and *.h). Many of these files are in the src directory itself. There are also dozens of "packages", which can be included or excluded when LAMMPS is built. See the doc/Section_build.html section of the manual for more information about packages, or type "make" from within the src directory, which lists package-related commands, such as "make package-status". The source files for each package are in an all-uppercase sub-directory of src, like src/MOLECULE or src/USER-CUDA. If the package is currently installed, copies of the package source files will also exist in the src directory itself. The src/STUBS sub-directory is not a package but contains a dummy version of the MPI library, used when building a serial version of the code.

The lib directory also contains source code for external libraries, used by a few of the packages. Each sub-directory, like meam or gpu, contains the source files, some of which are in different languages such as Fortran. The files are compiled into libraries from within each sub-directory, e.g. performing a "make" in the lib/meam directory creates a libmeam.a file. These libraries are linked to during a LAMMPS build, if the corresponding package is installed.

LAMMPS C++ source files almost always come in pairs, such as run.cpp and run.h. The pair of files defines a C++ class, the Run class in this case, which contains the code invoked by the "run" command in a LAMMPS input script. As this example illustrates, source file and class names often have a one-to-one correspondence with a command used in a LAMMPS input script. Some source files and classes do not have a corresponding input script command, e.g. force.cpp and the Force class. They are discussed in the next section.

2 Class hierarchy of LAMMPS

Though LAMMPS has a lot of source files and classes, its class hierarchy is quite simple, as outlined in Fig 1. Each boxed name refers to a class and has a pair of associated source files in lammps/src, e.g. memory.cpp and memory.h. More details on the class and its methods and data structures can be found by examining its *.h file.

LAMMPS (lammps.cpp/h) is the top-level class for the entire code. It holds an "instance" of LAMMPS and can be instantiated one or more times by a calling code. For example, the file src/main.cpp simply instantiates one instance of LAMMPS and passes it the input script.

The file src/library.cpp contains a C-style library interface to the LAMMPS class. See the lammps/couple and lammps/python directories for examples of simple programs that use LAMMPS through its library interface. A driver program can instantiate the LAMMPS class multiple times, e.g. to embed several atomistic simulation regions within a mesoscale or continuum simulation domain.

There are a dozen or so top-level classes within the LAMMPS class that are visible everywhere in the code. They are shaded blue in Fig 1. Thus any class can refer to the y-coordinate of local atom I as atom→x[i][1]. This visibility is enabled by a bit of cleverness in the Pointers class (see src/pointers.h) which every class inherits from.

There are a handful of virtual parent classes in LAMMPS that define what LAMMPS calls "styles". They are shaded red in Fig 1. Each of these are parents of a number of child classes that implement the interface defined by the parent class. For example, the fix style has around 100 child classes. They are the possible fixes that can be specified by the fix command in an input script, e.g. fix nve, fix shake, fix ave/time, etc. The corresponding classes are Fix (for the parent class), FixNVE, FixShake, FixAveTime, etc. The source files for these classes are easy to identify in the src directory, since they begin with the word "fix", e,g, fix_nve.cpp, fix_shake,cpp, fix_ave_time.cpp, etc.

The one exception is child class files for the "command" style. These implement specific commands in the input script that can be invoked before/after/between runs or which launch a simulation. Examples are the create_box, minimize, run, and velocity commands which encode the CreateBox, Minimize, Run, and Velocity classes. The corresponding files are create_box,cpp, minimize.cpp, run.cpp, and velocity.cpp. The list of command style files can be found by typing "grep COMMAND_CLASS *.h" from within the src directory, since that word in the header file identifies the class as an input script command. Similar words can be grepped to list files for the other LAMMPS styles. E.g. ATOM_CLASS, PAIR_CLASS, BOND_CLASS, REGION_CLASS, FIX_CLASS, COMPUTE_CLASS, DUMP_CLASS, etc.

More details on individual classes in Fig 1 are as follows:

- The Memory class handles allocation of all large vectors and arrays.
- The Error class prints all error and warning messages.

- The Universe class sets up partitions of processors so that multiple simulations can be run, each on a subset of the processors allocated for a run, e.g. by the mpirun command.
- The Input class reads an input script, stores variables, and invokes standalone commands that are child classes of the Command class.
- As discussed above, the Command class is a parent class for certain input script commands that perform a one-time operation before/after/between simulations or which invoke a simulation. They are instantiated from within the Input class, invoked, then immediately destructed.
- The Finish class is instantiated to print statistics to the screen after a simulation is performed, by commands like run and minimize.
- The Special class walks the bond topology of a molecular system to find 1st, 2nd, 3rd neighbors of each atom. It is invoked by several commands, like read_data, read_restart, and replicate.
- The Atom class stores all per-atom arrays. More precisely, they are allocated and stored by the AtomVec class, and the Atom class simply stores a pointer to them. The AtomVec class is a parent class for atom styles, defined by the atom_style command.
- The Update class holds an integrator and a minimizer. The Integrate class is a parent style for the Verlet and rRESPA time integrators, as defined by the run_style input command. The Min class is a parent style for various energy minimizers.
- The Neighbor class builds and stores neighbor lists. The NeighList class stores a single list (for all atoms). The NeighRequest class is called by pair, fix, or compute styles when they need a particular kind of neighbor list.
- The Comm class performs interprocessor communication, typically of ghost atom information. This usually involves MPI message exchanges with 6 neighboring processors in the 3d logical grid of processors mapped to the simulation box. Sometimes the Irregular class is used, when atoms may migrate to arbitrary processors.
- The Domain class stores the simulation box geometry, as well as geometric Regions and any user definition of a Lattice. The latter are defined by region and lattice commands in an input script.
- The Force class computes various forces between atoms. The Pair parent class is for non-bonded or pair-wise forces, which in LAMMPS lingo includes many-body forces such as the Tersoff 3-body potential. The Bond, Angle, Dihedral, Improper parent classes are styles for bonded interactions within a static molecular topology. The KSpace parent class is for

computing long-range Coulombic interactions. One of its child classes, PPPM, uses the FFT3D and Remap classes to communicate grid-based information with neighboring processors.

- The Modify class stores lists of Fix and Compute classes, both of which are parent styles.
- The Group class manipulates groups that atoms are assigned to via the group command. It also computes various attributes of groups of atoms.
- The Output class is used to generate 3 kinds of output from a LAMMPS simulation: thermodynamic information printed to the screen and log file, dump file snapshots, and restart files. These correspond to the Thermo, Dump, and WriteRestart classes respectively. The Dump class is a parent style.
- The Timer class logs MPI timing information, output at the end of a run.

3 How a timestep works

The first and most fundamental operation within LAMMPS to understand is how a timestep is structured. Timestepping is performed by the Integrate class within the Update class. Since Integrate is a parent class, corresponding to the run_style input script command, it has child classes. In this section, the timestep implemented by the Verlet child class is described. A similar timestep is implemented by the Respa child class, for the rRESPA hierarchical timestepping method. The Min parent class performs energy minimization, so does not perform a literal timestep. But it has logic similar to what is described here, to compute forces and invoke fixes at each iteration of a minimization. Differences between time integration and minimization are highlighted at the end of this section.

The Verlet class is encoded in the src/verlet.cpp and verlet.h files. It implements the velocity-Verlet timestepping algorithm. The workhorse method is Verlet::run(), but first we highlight several other methods in the class.

- The init() method is called at the beginning of each dynamics run. It simply sets some internal flags, based on user settings in other parts of the code.

- The setup() or setup_minimal() methods are also called before each run. The velocity-Verlet method requires current forces be calculated before the first timestep, so these routines compute forces due to all atomic interactions, using the same logic that appears in the timestepping described next. A few fixes are also invoked, using the mechanism described in the next section. Various counters are also initialized before the run begins. The setup_minimal() method is a variant that has a flag for performing less setup. This is used when runs are continued and information from the previous run is still valid. For example, if repeated short LAMMPS runs are being invoked, interleaved by other commands, via the "pre no" and "every" options of the run command, the setup_minimal() method is used.

- The force_clear() method initializes force and other arrays to zero before each timestep, so that forces (torques, etc) can be accumulated.

Now for the Verlet::run() method. Its structure in hi-level pseudo code is shown in Fig 2. In the actual code in src/verlet.cpp some of these operations are conditionally invoked.

The ev_set() method (in the parent Integrate class), sets two flags (*eflag* and *vflag*) for energy and virial computation. Each flag encodes whether global and/or per-atom energy and virial should be calculated on this timestep, because some fix or variable or output will need it. These flags are passed to the various methods that compute particle interactions, so that they can skip the extra calculations if the energy and virial are not needed. See the comments with the Integrate::ev_set() method which document the flag values.

At various points of the timestep, fixes are invoked, e.g. fix→initial_integrate(). In the code, this is actually done via the Modify class which stores all the Fix objects and lists of which should be invoked at what point in the timestep. Fixes are the LAMMPS mechanism for tailoring the operations of a timestep for a particular simulation. As described elsewhere (unwritten section), each fix has one or more methods, each of which is invoked at a specific stage of the timestep, as in Fig 2. All the fixes defined in an input script with an initial_integrate() method are invoked at the beginning of each timestep. Fix nve, nvt, npt are examples, since they perform the start-of-timestep velocity-Verlet integration to update velocities by a half-step, and coordinates by a full step. The post_integrate() method is next. Only a few fixes use this, e.g. to reflect particles off box boundaries in the FixWallReflect class.

The decide() method in the Neighbor class determines whether neighbor lists need to be rebuilt on the current timestep. If not, coordinates of ghost atoms are acquired by each processor via the forward_comm() method of the Comm class. If neighbor lists need to be built, several operations within the inner if clause of Fig 2 are first invoked. The pre_exchange() method of any defined fixes is invoked first. Typically this inserts or deletes particles from the system.

Periodic boundary conditions are then applied by the Domain class via its pbc() method to remap particles that have moved outside the simulation box back into the box. Note that this is not done every timestep. but only when neighbor lists are rebuilt. This is so that each processor's sub-domain will have consistent (nearby) atom coordinates for its owned and ghost atoms. It is also why dumped atom coordinates can be slightly outside the simulation box.

The box boundaries are then reset (if needed) via the reset_box() method of the Domain class, e.g. if box boundaries are shrink-wrapped to current particle coordinates. A change in the box size or shape requires internal information for communicating ghost atoms (Comm class) and neighbor list bins (Neighbor class) be updated. The setup() method of the Comm class and setup_bins() method of the Neighbor class perform the update.

The code is now ready to migrate atoms that have left a processor's geometric sub-domain to new processors. The exchange() method of the Comm class performs this operation. The borders() method of the Comm class then identifies ghost atoms surrounding each processor's sub-domain and communicates ghost atom information to neighboring processors. It does this by looping over all the atoms owned by a processor to make lists of those to send to each neighbor processor. On subsequent timesteps, the lists are used by the Comm::forward_comm() method.

Fixes with a pre_neighbor() method are then called. These typically re-build some data structure stored by the fix that depends on the current atoms owned by each processor.

Now that each processor has a current list of its owned and ghost atoms, LAMMPS is ready to rebuild neighbor lists via the build() method of the Neighbor class. This is typically done by binning all owned and ghost atoms, and scanning a stencil of bins around each owned atom's bin to make a Verlet list of neighboring atoms within the force cutoff plus neighbor skin distance.

In the next portion of the timestep, all interaction forces between particles are computed, after zeroing the per-atom force vector via the force_clear() method. If the newton flag is set to "on" by the newton command, forces on both owned and ghost atoms are calculated.

Pairwise forces are calculated first, which enables the global virial (if requested) to be calculated cheaply (at the end of the Pair::compute() method), by a dot product of atom coordinates and forces. By including owned and ghost atoms in the dot product, the effect of periodic boundary conditions is correctly accounted for. Molecular topology interactions (bonds, angles, dihedrals, impropers) are calculated next. The final contribution is from long-range Coulombic interactions, invoked by the KSpace class.

If the newton flag is on, forces on ghost atoms are communicated and summed back to their corresponding owned atoms. The reverse_comm() method of the Comm class performs this operation, which is essentially the inverse operation of sending copies of owned atom coordinates to other processor's ghost atoms.

At this point in the timestep, the total force on each atom is known. Additional force constraints (external forces, SHAKE, etc) are applied by Fixes that have a post_force() method. The second half of the velocity-Verlet integration is then performed (another half-step update of the velocities) via fixes like nve, nvt, npt.

At the end of the timestep, fixes that define an end_of_step() method are invoked. These typically perform a diagnostic calculation, e.g. the ave/time and ave/spatial fixes. The final operation of the timestep is to perform any requested output. There are 3 kinds of LAMMPS output: thermodynamic output to the screen and log file, snapshots of atom data to a dump file, and restart files. See the thermo_style, dump, and restart commands for more details.

The iteration performed by an energy minimization is similar to the dynamics timestep of Fig 2. Forces are computed, neighbor lists are built as needed, atoms migrate to new processors, and atom coordinates and forces are communicated to neighboring processors. The only difference is what Fix class operations are invoked when. Only a subset of LAMMPS fixes are useful during energy minimization, as explained in their individual doc pages. The relevant Fix class methods are min_pre_exchange(), min_pre_force(), and min_post_force(). Each is invoked at the appropriate place within the minimization iteration. For example, the min_post_force() method is analogous to the post_force() method for dynamics; it is used to alter or constrain forces on each atom, which affects the minimization procedure.

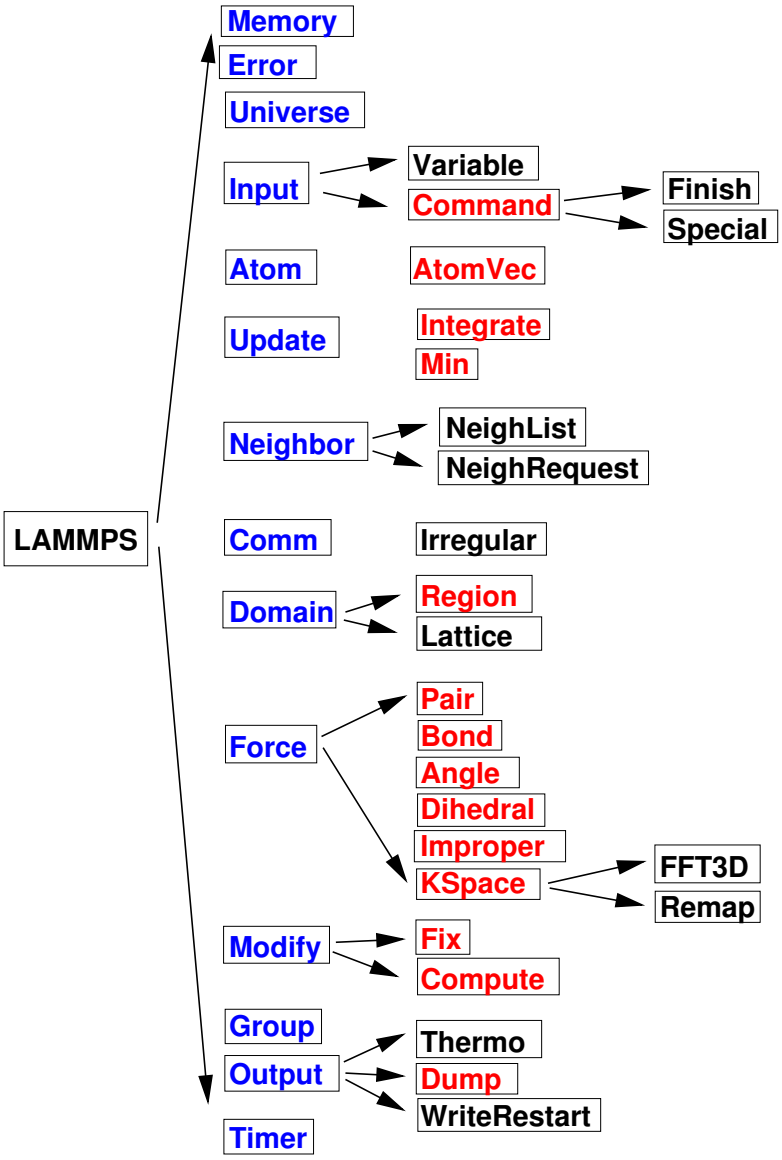

Figure 1: Class hierarchy in LAMMPS source code.

```
loop over N timesteps:
  ev_set()

  fix->initial_integrate()
  fix->post_integrate()

  nflag = neighbor->decide()
  if nflag:
    fix->pre_exchange()
    domain->pbc()
    domain->reset_box()
    comm->setup()
    neighbor->setup_bins()
    comm->exchange()
    comm->borders()
    fix->pre_neighbor()
    neighbor->build()
  else
    comm->forward_comm()

  force_clear()
  fix->pre_force()

  pair->compute()
  bond->compute()
  angle->compute()
  dihedral->compute()
  improper->compute()
  kspace->compute()

  comm->reverse_comm()

  fix->post_force()
  fix->final_integrate()
  fix->end_of_step()

  if (any output on this step) output()
```

Figure 2: Pseudo-code for Verlet::run() method.