Modifying & Extending LAMMPS

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Resources for modifying LAMMPS

- Before you start writing code:
  - be familiar with what is already in LAMMPS
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- search the mail list
  - http://lammps.sandia.gov/mail.html
  - google: lammps-users thermostat Lowe
    1st hit: lammps.sandia.gov/threads/msg20748.html
    2nd hit: SourceForge.net: LAMMPS: lammps-users
    Ad hit: Thermostats at Lowe’s (www.lowes.com)
- post a “how can I do this” message to the mail list
  - email to lammps-users@lists.sourceforge.net
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Section in manual: Modifying & Extending LAMMPS
- doc/Section_modify.html
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Section in manual: Modifying & Extending LAMMPS

- doc/Section_modify.html

Developers manual (brief!)

- doc/Developer.pdf
- diagram of class hierarchy
- pseudo-code & explanation of how a timestep works
LAMMPS itself is a class
- can be instantiated multiple times
- has library interface
- callable via C++, C, Fortran, Python

Blue are core classes
- visible anywhere in LAMMPS

Red are style classes
- one parent class
- many child classes
Rule of thumb: every input script command has corresponding class and corresponding file name
- run command ⇒ Run class ⇒ run.cpp + run.h
- pair_style lj/cut command ⇒ PairLJCut class ⇒ pair_lj_cut.cpp/h

Src directory
- core classes are all here
- many style classes also here

Package sub-directories (type make package to see)
- package = group of related style classes
- src/KSPACE = long-range Coulombic solvers
- src/USER-OMP = OpenMP versions of many classes (Axel)
  - two flavors: standard (26) and user (13)

Lib directory
- some packages require auxiliary libraries
- those included in LAMMPS are under lib
- examples: lib/gpu, lib/meam, lib/colvars (Axel)
Core classes

See doc/Developer.pdf for more details

- **Memory** = memory allocation of 1d, 2d, etc arrays
- **Error** = error and warning messages
- **Universe** = partition procs ⇒ multiple “worlds”, one per sim
- **Input** = read input script, variables, added commands
- **Atom** = per-particle data
- **Update** = dynamics and minimization
- **Neighbor** = build neighbor lists
- **Comm** = inter-processor communication
- **Domain** = simulation box and geometric regions
- **Force** = potentials (pair, bond, angle, etc, KSpace)
- **Modify** = fixes and computes
- **Group** = collections of particles
- **Output** = thermodynamics, dump files, restart files
- **Timer** = timings statistics

Look at header files (src/domain.h) to understand core classes and LAMMPS generally
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90% of source code is extensions via 14 styles
See src/style*.h or grep CLASS *.h
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Easy for developers and users to add new features:
- particle types = atom style
- force fields = pair, bond, angle, dihedral, improper styles
- long range = kspace style
- fix = fix style = BC, constraint, time integration, ...
- diagnostics = compute style
- geometric region = region style
- integrator = integrate style (Verlet, rRESPA)
- minimizer = min style
- snapshot output =
- dump style
- input command = command style = read_data, velocity, run
Other code details

- **Pointers** = ultimate base class
  - all classes (except LAMMPS) derive from it
  - holds pointers to all core classes
  - enables easy access anywhere in code
    - domain→xprd for x box-length
- Everything inside **LAMMPS_NS namespace**
  - no external (global) variables
  - allows multiple instantiations of LAMMPS
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- **MPI communicators**
  - pass in from `main()` or thru library interface as `world`
    - enables a LAMMPS instantiation to run on any set of procs
  - `universe` class partitions allocation into multiple worlds
    - enables multiple simulations to run simultaneously

- **C++ vs Fortran**
  - pre-2004 LAMMPS was in Fortran
  - re-wrote in C++ for flexibility in adding new features
  - very little fancy C++ (templating, STL, etc)
  - core kernels are C-like, so coding style is really OO C
4 ways to extend LAMMPS

1. Add new styles
   - sky is the limit!

2. Add code to existing files

3. Add new fields to data file as atom properties

4. Add methods to the library interface
   - really “extending” external to LAMMPS
Again, 90% of source code is extensions via 14 styles

- Enabled by C++
  - virtual parent class defines interface rest of LAMMPS uses
  - style = new child class implementing a few methods
Extending LAMMPS via styles

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- In theory:
  - just add new *.cpp and *.h file to src and re-compile
  - your new class will work with all LAMMPS functionality
  - your new class won’t break anything else
  - in practice, theory and practice are not always the same
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Now discuss nuts & bolts, then show 5 examples
How to write a new style

See `doc/Section_modify.html` for overview and key methods
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- Find an existing style that does something similar
  - ask on mail list or send developers an email
  - especially important if you want to do something complex
    - does functionality you want already exist?
    - is it a good idea to do this in LAMMPS?
    - will it be parallel?
    - can advise you as to possible gotchas
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- Decide which style is most appropriate
  - **computes** calculate at one timestep
  - **fixes** can alter something during timestep
  - **fixes** can maintain info from timestep to timestep
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  - **computes** calculate at one timestep
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- Understand **how that style works** and is structured
  - examine parent class header file (e.g. `pair.h`)
  - learn what methods it supports (`doc/Section_modify.html`)
  - look at other `*.cpp` and `*.h` files of that style
  - if you get stuck, post to mail list
How to write a new pair style

Find a similar pair style ...

- **Flags** in constructor: see pair.h
  - manybody_flag, single_enable, respa_enable, comm_forward, etc
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- **compute()** method
  - loop over atoms and neighbors
  - calculate energy and forces
- **settings()** method
  - pair_style lj/cut cutoff
- **coeff()** method
  - pair_coeff I J epsilon sigma
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- **coeff()** method
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- **init_one()** method
  - pre-compute all needed factors, symmetrize I,J = J,I
- **write_restart()** and **read_restart()** methods
- **single()** method
  - energy/force for one I,J pair of particles
How to write a new compute style

Find a similar compute ...

- What will the compute produce?
  - global or per-atom or local values
  - scalar or vector or array
  - see `doc/Section_howto 6.15`
  - see compute.h for what flags to set
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  - global or per-atom or local values
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- Corresponding methods to implement:
  - `compute_scalar()` = single global value
    - compute temp
  - `compute_vector()` = few values
    - compute group/group for force components
  - `compute_array()` = array of few values like
    - compute rdf
  - `compute_peratom()` = one or more values per atom
    - compute coord/atom, compute displace/atom
  - `compute_local()` = one or more values per pair, bond, etc
    - compute pair/local, compute bond/local
Fixes allow tailoring of timestep

In hindsight, best feature of LAMMPS for flexibility
Allows control of what happens when within each timestep

Loop over timesteps:

- communicate ghost atoms
- build neighbor list (once in a while)
- compute forces
- communicate ghost forces

output to screen and files
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Allows control of what happens when within each timestep

Loop over timesteps:
  fix initial NVE, NVT, NPT, rigid-body integration
  communicate ghost atoms
  fix neighbor insert particles
  build neighbor list (once in a while)
  compute forces
  communicate ghost forces
  fix force SHAKE, langevin drag, wall, spring, gravity
  fix final NVE, NVT, NPT, rigid-body integration
  fix end volume & T rescaling, diagnostics
  output to screen and files
How to write a new fix style

Find a similar fix ...

- setmask() method, e.g. for fix nve:
  
  ```c
  int mask = 0;
  mask |= INITIAL_INTEGRATE;
  mask |= FINAL_INTEGRATE;
  return mask;
  ```

Corresponding methods to implement:
- initial integrate()
- pre exchange()
- post force()
- final integrate()
- end of step()
- fix deform, fix ave/time = change system, diagnostics
How to write a new fix style

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- **setmask()** method, e.g. for fix nve:
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- **Corresponding methods to implement:**
  - **initial_integrate()**
    - fix nvt, nvt, npt, rigid = first half of Verlet update
  - **pre_exchange()**
    - fix deposit, evaporate = insert, remove particles
  - **post_force()**
    - fix addforce, shake, fix wall = adjust or constrain forces
  - **final_integrate()**
    - second half of Verlet update
  - **end_of_step()**
    - fix deform, fix ave/time = change system, diagnostics
Fixes can ...

- request a neighbor list (so can compute)
- perform ghost-atom communication (so can compute)
- store values that migrate with atoms
  - `grow_arrays()`, `copy_arrays()`, `pack_exchange()`, `unpack_exchange()`
- write/read info to/from restart file
  - fix nvt (global), fix store/state (per-atom)
Fixes can ...

- request a **neighbor list** (so can compute)
- perform **ghost-atom communication** (so can compute)
- store values that migrate with atoms
  - grow_arrays(), copy_arrays(), pack_exchange(), unpack_exchange()
- write/read info to/from **restart file**
  - fix nvt (global), fix store/state (per-atom)

Will the fix produce any **output**?

- global or per-atom or local values
  - fix nvt stores thermostat energy contribution
- scalar or vector or array
- see **doc/Section_howto 6.15**
- same flags to set in fix.h
How to write a new atom style

Don’t do it, if can avoid it ...

- See new `fix property/atom` command
  - add a molecule ID to style without one
    - example: treat granular clusters as rigid bodies
    - instead of `atom_style hybrid sphere bond`
  - add arbitrary `i_myflag, d_sx d_sy d_sz`
  - access the per-atom values in other classes

See new `atom_style body` command
useful for “particles” with internal state
example: aspherical particle with sub-particles
example: aspherical particle with surface grid
end up writing a small body style, not a large atom style
see doc/body.html for details
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If you really need to write a new atom style (advanced)

Study an existing atom style ...

- **Flags** in constructor: see `atom_vec.h`
  - molecular, mass_type, size_forward, size_data_atom, etc
If you really need to write a new atom style (advanced)

Study an existing atom style ...

- **Flags** in constructor: see atom_vec.h
  - molecular, mass_type, size_forward, size_data_atom, etc
- **grow()** method - allocates all per-atom arrays
- **(un)pack_comm()** method - communicate every step
- **(un)pack_border()** method - communicate every re-neighbor
- **(un)pack_exchange()** method - migrate info with atom
- **create_atom()** method - create one atom
- **data_atom()** method - read atom from data file
If you really need to write a new atom style (advanced)

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- **create_atom()** method - create one atom
- **data_atom()** method - read atom from data file
- And a dozen others …
  - variants to work in atom_style hybrid mode
Questions?

Take a break and stretch ...
Five examples of LAMMPS style extensions

- Triangular regions: region tri
- Molecule size/shape: compute rg/molecule
- Solvent evaporation: fix evaporate
- Grain boundary migration: fix orient/fcc
- Shock-induced explosive detonation: fix wall/reflect
#1 - Triangular regions

- Derived class: `RegionTri` in `region_tri.cpp/h`
- Header file:
  ```
  #ifdef REGION_CLASS
  RegionStyle(tri,RegTri)
  #else
  
  Input script syntax: (just for 2d problems)
  ```
  ```
  region bump tri x1 y1 x2 y2 x3 y3
  ```
- `RegionTri(int narg, char **arg)`
  ```
  reads arguments: x1 y1 x2 y2 x3 y3
  ```
  ```
  determines bounding box
  ```
- `inside(double x, double y, double z) method`
  ```
  determine if (x,y) is inside triangle
  ```
  ```
  3 positive cross products ⇒ inside
  ```
- ~35 lines of code
Friction example

Substitute (twice):
region lo-asperity sphere 32 7 0 8
region lo-asperity tri 26 7 32 14 38 7
Stick-slip flow on corrugated surfaces
Nikolai Priezjev group at Michigan State U

Flow is function of corrugation wavelength and chain length
Monitor shape and motion of chains
Compute gyration/molecule for $R_g$ of each polymer chain

- **Input script:**
  ```
  compute id all gyration/molecule {tensor}
  compute_vector() method (40 lines, one value/molecule):
  ```
  ```for (int i = 0; i < nlocal; i++)
  if (mask[i] & groupbit) {
    imol = molecule[i];
    domain->unmap(x[i], image[i], unwrap);
    dx = unwrap[0] - comall[imol][0];
    dy = unwrap[1] - comall[imol][1];
    dz = unwrap[2] - comall[imol][2];
    massone = mass[type[i]];
    rg[imol] += (dx*dx + dy*dy + dz*dz) * massone;
  }
  MPI_Allreduce(rg, vector, nmolecules,...);
  ```
Compute gyration/molecule for $R_g$ of each polymer chain

- Input script:
  ```
  compute id all gyration/molecule {tensor}
  compute vector() method (40 lines, one value/molecule):
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  ```c
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    if (mask[i] & groupbit) {
      imol = molecule[i];
      domain->unmap(x[i], image[i], unwrap);
      dx = unwrap[0] - comall[imol][0];
      dy = unwrap[1] - comall[imol][1];
      dz = unwrap[2] - comall[imol][2];
      massone = mass[type[i]];
      rg[imol] += (dx*dx + dy*dy + dz*dz) * massone;
    }
  MPI_Allreduce(rg,vector,nmolecules,...);
  ```

- For shape, compute inertia/molecule is similar logic
#3 - Solvent evaporation

- Nanoparticle ordering in polymers w/ solvent evaporation
- Spring MRS meeting, 2013

- Evaporate solvent at controlled rate above L/V interface
- Ordering is function of NP/polymer interaction strength
Fix evaporate removes solvent at specified rate

- **Input script:**
  ```
  fix id solvent evaporate
  N M topbox 38277 {molecule yes}
  ```
- **pre_exchange() method**

  - identify atoms in region volume
  - pick random subset (consistent across procs)
  - delete from system
  - also remove molecules the deleted particles are in

- ~200 lines of code (molecules add some complexity)
Add synthetic energy/force as function of mis-orientation
Drives atoms near boundary from orientation I to J
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Drives atoms near boundary from orientation I to J
Mobility $\propto$ migration velocity / driving force
Extract accurate mobility from short simulation
Build a bi-crystal

Input script commands:

```
region lower box EDGE EDGE EDGE EDGE EDGE EDGE 20.0
region upper box EDGE EDGE EDGE EDGE EDGE EDGE 20.0 EDGE
lattice fcc 4.04 origin 0 20 0 orient x -3 1 0 ...
create_atoms 1 region lower
lattice fcc 4.04 origin 0 20 0 orient x 3 1 0 ...
create_atoms 1 region upper
delete_atoms overlap 0.5 all all
```
Fix orient/fcc to impose driving force

- 2 files: src/fix_orient_fcc.cpp and fix_orient_fcc.h
- Request **full neighbor list**, every timestep:

```c
int irequest = neighbor->request((void *) this);
neighbor->requests[irequest]->pair = 0;
neighbor->requests[irequest]->fix = 1;
neighbor->requests[irequest]->half = 0;
neighbor->requests[irequest]->full = 1;
```
Post_force() method for fix orient/fcc

double loop over atoms and neighbors:
  compute $R_{ij}$ and add to list
  sort list to find 12 nearest neighbors (fcc)

loop over atoms:
  compute contributions from 12 neighbors
  derivative of energy $\rightarrow$ forces on I and J atoms

communicate partial forces induced on ghost atoms

double loop over atoms and neighbors:
  compute full orientation force on each I atom
Post_force() method for fix orient/fcc

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communicate partial forces induced on ghost atoms

double loop over atoms and neighbors:
  compute full orientation force on each I atom

- LAMMPS provides method to perform communication
- $\sim$250 lines of code
**#5 - Shock-induced detonation of explosives**

- *R Shan & A Thompson, March APS meeting (2013)*
- **PETN** is a powerful high explosive
- Simulate “slow” shock wave passing thru PETN crystal
- *R Shan & A Thompson, March APS meeting (2013)*
- **PETN** is a powerful high explosive
- Simulate “slow” shock wave passing thru PETN crystal
- Use a *reactive force field* (ReaxFF)
  - detonation is triggered by onset of exothermic reactions
- Quantify detonation **sensitivity** to orientation, defects, impurities ... a safety issue
Create a void in PETN crystal

Input script commands:

- read_data data.petn.molecule
- replicate 100 50 50
- region void sphere 20.0 30.0 30.0 5.0
- delete_atoms all region void
Largest void size = 20 nm

8.9M atoms (60x40x40 nm)
10 psec (20K steps, 100 hours on 4096 cores)
Post\_integrate() method for fix wall/reflect command

```c
for (int m = 0; m < nwall; m++)
    coord = current wall position (fixed or variable)
    dim = wallwhich[m] / 2; side = wallwhich[m] % 2;

for (i = 0; i < nlocal; i++)
    if (side == 0)
        if (x[i][dim] < coord)
            x[i][dim] = coord + (coord - x[i][dim]);
            v[i][dim] = -v[i][dim];
        else
            if (x[i][dim] > coord)
                x[i][dim] = coord - (x[i][dim] - coord);
                v[i][dim] = -v[i][dim];
```
Post_integrate() method for fix wall/reflect command

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- Entire fix = ~200 lines of code
Fix reaxc/species command for molecule statistics

- Written by Ray Shan (Sandia)
- Molecules in ReaxFF and a shock explosion are dynamic
  - not defined by permanent bonds, angles, etc
  - defined by instantaneous bond-order parameters
- Useful to know numbers/locations/atoms of molecules at any timestep, on-the-fly
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- Compute cluster/atom flags clusters based on cutoff
  - each atom starts as own cluster
  - walk outward, merging clusters with lower atom ID
  - parallel communication when clusters overlap proc domains
- Use same logic to merge based on bond-order criterion
- Compile molecule stats and write details to file
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- Compile molecule stats and write details to file
- Entire fix = $\sim$1000 lines of code
Extending LAMMPS by adding to existing files

3 cases where this is straight-forward:

1. Adding keywords to thermo style output
   
   see thermo.cpp

2. Adding new functions to equal-style and atom-style variables

   see variable.cpp
   
   math functions, special functions, math operators, etc

   make sure you follow syntax rules for args of similar functions

3. Adding keywords for per-atom fields

   only needed if write new atom style

   see compute

   property

   atom.cpp

   allows use of field in all other commands

   dump, fix ave/spatial, atom-style variables, etc

In each case, look for customize comments in appropriate src file
3 cases where this is straight-forward:

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Extending LAMMPS by adding to existing files

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3. Adding keywords for per-atom fields
   - only needed if write new atom style
   - see compute_property_atom.cpp
   - allows use of field in all other commands
     - dump, fix ave/spatial, atom-style variables, etc
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In each case, look for customize comments in appropriate src file
Adding new fields to data file (advanced)

- New **header lines** and/or **new sections**
  - 1500 multistates
  - Multistates
  - 1 27 ...
  - ...
  - 1500 13 ...
- Previously required extensions to read_data.cpp
Adding new fields to data file (advanced)

- New **header lines** and/or **new sections**
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- Previously required extensions to `read_data.cpp`

- Can now be done in a fix
  - `read_data data.poly fix ID multistates Multistates ...`
  - can read from data file and store per-atom info
  - virtual void `read_data_header(char *)`;
  - virtual void `read_data_section(char *, int, char *)`;
  - virtual bigint `read_data_skip_lines(char *)`;
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- See **fix property/atom** for a working example
- **CMAP** 5-body interactions are being implemented this way
Using LAMMPS thru its library interface

See Section _howto_.html 6.19 and Section _python_.html in manual
See _src/library.cpp_ and _src/library.h_

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

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

See examples/COUPLE/simple for C, C++, Fortran
See python/examples for Python, Pizza.py for GnuPlot wrapper

```python
%% python plot.py in.lammps Nfreq Nsteps compute-ID

from gnu import gnu
from lammps import lammps
lmp = lammps()
lmp.file(infile)
lmp.command("thermo %d" % Nfreq)

lmp.command("run 0 pre yes post no")
value = lmp.extract_compute(computeID,0,0)
ntimestep = 0
xaxis = [ntimestep]
yaxis = [value]
```
if me == 0:
    gn = gnu()
    gn.plot(xaxis,yaxis)
    gn.xrange(0,nsteps)
    gn.title(computeID,"Timestep","Temperature")

while ntimestep < Nsteps:
    lmp.command("run %d pre no post no" % Nfreq)
    ntimestep += nfreq
    value = lmp.extract_compute(computeID,0,0)
    xaxis.append(ntimestep)
    yaxis.append(value)
    if me == 0:  gn.plot(xaxis,yaxis)

lmp.command("run 0 pre no post yes")
What it produces, in real time

This includes GUI slider & dump output to Pizza.py GL tool (or AtomEye or Pymol or VMD) - see python/examples scripts
Again, see library.cpp and library.h

- **Accessor functions** already exist for ...
  - system variables (box, timestep, etc)
  - per-atom pointers (x, v, etc)
  - compute and fix output
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Extending the LAMMPS library interface

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- **New functions** in library.cpp can ...
  - access any public data within LAMMPS
  - invoke any public methods of any classes

- **New functions** are limited only by your imagination!
Most important class to understand: Verlet ⇒ src/verlet.cpp
How a timestep works - part 1

Most important class to understand: Verlet ⇒ src/verlet.cpp

Look at the run() method (in 3 parts)
See doc/Developer.pdf for more details

loop over N timesteps:
  ev_set()
  fix->initial_integrate()
  fix->post_integrate()
  ...

loop over N timesteps:
...
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()
...
How a timestep works - part 3

loop over N timesteps:
   ...
   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->write()
How to get your code added to the LAMMPS distro

Mail it to us, but first ...

- see doc/Section_modify.html
- sub-section: Submitting new features for inclusion in LAMMPS
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- **Why release** it as part of main LAMMPS?
  - open source philosophy  
  - fame and fortune, name on author page and in source code  
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    - find and fix bugs  
    - extend its functionality  
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- Must provide a doc page as a *.txt file
  - one for every command that appears in input script
  - see similar doc/*/*.txt file as starting point
  - if needed, equations for doc/Eqs as LaTeX files
  - we auto-convert to HTML (and JPG if needed)
How to get your code added (continued)

- **Rule:** don’t make changes in core of LAMMPS
  1. if you think you need to, talk to developers
  2. the more I need to think, the longer it will take to release

- **Suggestion:** write your code in the LAMMPS format
  1. easier for everyone to read, maintain
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- **USER-MISC package**
  1. if it compiles, we’ll add it (within limits)
  2. don’t really care if written in LAMMPS format
  3. you own it, answer Qs, and update it
  4. set of related commands can be an entire USER package

- **Commands that link to an external library**
  1. must become a package (standard or user)
  2. type “make package” for list
What features do you need for your models?

Happy to brainstorm & discuss this week