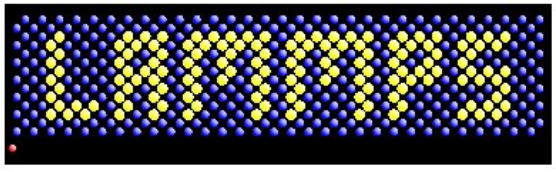
How to modify LAMMPS

Steve Plimpton
Sandia National Labs
sjplimp@sandia.gov

7th LAMMPS Workshop and Symposium
Virtual meeting – August 2021



Center for Computing Research

Sandia National Laboratories

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

National Nuclear Security Administration

You have an idea for a new LAMMPS feature

Questions to think about:

1. Does LAMMPS already have a similar feature ?
2. Have others discussed or worked on this before ?
3. Better done outside or inside LAMMPS ?
4. Can it be done with Python ?
5. Do you need help implementing the new feature ?
6. Is this just for you, or to contribute to public LAMMPS ?

(1) Does LAMMPS already have a similar feature ?

If yes ...

- Maybe it's sufficient for what you need
- Maybe it can be incrementally extended
- Maybe its code will show you how to implement your feature

(1) Does LAMMPS already have a similar feature ?

If yes ...

- Maybe it's sufficient for what you need
- Maybe it can be incrementally extended
- Maybe its code will show you how to implement your feature

Check the LAMMPS website and manual:

- Website has Google search bar $\Rightarrow$ website + manual
- Website has glossary MD $\Rightarrow$ LAMMPS page
- Website has Commands page (part of manual)
  - alphabetized tables for pair styles, fixes, computes, etc
  - fix command doc page has one-line description of each
  - ditto for compute and pair_style command doc pages
- Manual webpages have Search docs option at top left
- Google "LAMMPS whatever" and find stuff

(2) Have others discussed or worked on this before ?

3 places you can look:

- Mail list
  - 80K+ messages
  - website Mail list page: info on posting and searching
  - Google search with lammps-users
- MatSci forum
  - new umbrella site for many materials modeling codes
  - website Matsci forum page: info on joining and browsing
- GitHub issues
  - GitHub site: `https://github.com/lammps/lammps`
  - Issues link at at top of page
  - some "issues" are brainstorming for a new idea

(2) Have others discussed or worked on this before ?

3 places you can look:

- Mail list
  - 80K+ messages
  - website Mail list page: info on posting and searching
  - Google search with lammps-users
- MatSci forum
  - new umbrella site for many materials modeling codes
  - website Matsci forum page: info on joining and browsing
- GitHub issues
  - GitHub site: `https://github.com/lammps/lammps`
  - Issues link at at top of page
  - some "issues" are brainstorming for a new idea

If don't find anything, you can ask a Q on mail list or forum
Good to give big picture of what you want to do
May be already possible in ways you haven't thought about

(3) Better done outside or inside LAMMPS ?

Generally outside:

- Pre- or post-processing tasks ⇒ website Pre/Post tools page
- Complex operations only loosely coupled to LAMMPS
  1. invoke external program from LAMMPS input script
     - data exchange thru files LAMMPS already knows how to read
     - shell command invokes, existing LAMMPS command reads
     - could be an existing program that writes in LAMMPS format
     - could be a new program you write
  2. client/server coupling
     - data volume is modest, exchange by single procs
     - two independent codes, e.g. for AIMD or QM/MM
     - see Section 8.8, Howto MDI in manual
  3. wrap an external library with new LAMMPS code
     - data volume is large, exchange in parallel thru lib API
     - compute voronoi/atom, pair KIM, pair quip, ...

Better done outside or inside LAMMPS ?

Generally inside:

- New feature invoked during timestepping
  - pair styles, fixes, computes
- Performance bottleneck if not parallel
- Needs to be coded in C++ for speed

(4) Can it be done with Python ?

- Often quicker to try something out, debug it in Python
- Maybe you only need to use the new code once
- Python may be fast enough $\Rightarrow$ no need to write C++ code
- Python can run in parallel via mpi4py, just like LAMMPS

(4) Can it be done with Python ?

- Often quicker to try something out, debug it in Python
- Maybe you only need to use the new code once
- Python may be fast enough $\Rightarrow$ no need to write C++ code
- Python can run in parallel via mpi4py, just like LAMMPS

Many ways to use Python with LAMMPS:

- Next: Richard Berger 30 min talk on this topic ...
- Python script wraps LAMMPS as a library
  - invoke LAMMPS input script commands
  - send, extract, and/or change internal LAMMPS data
  - LAMMPS can call back to Python
- Use input script python variable $\Rightarrow$ invoke Python function
- Fix python and pair_style python commands

So now you're going to add C++ code to LAMMPS

For big picture of how LAMMPS is structured:
new Programmer Guide recently added to manual

- Consolidates info scattered previously around User Guide
- New material recently added
- Section 3: Modifying & extending LAMMPS
  - next slide !
- Section 4: Information for Developers
  - class hierarchy (fairly simple and flat)
  - how a timestep works
  - various utility functions and classes

You're likely going to write code for a new style

- LAMMPS lingo: style = child class derived from a parent class
- More than 90% of LAMMPS code base is added styles
- Modifying & extending LAMMPS in Programmer Guide
  - mostly about styles
  - read the overview + sub-section for style you are adding

You're likely going to write code for a new style

- LAMMPS lingo: style = child class derived from a parent class
- More than 90% of LAMMPS code base is added styles
- Modifying & extending LAMMPS in Programmer Guide
  - mostly about styles
  - read the overview + sub-section for style you are adding
- Styles discussed:
  - atom style = per-particle data
  - pair style = particle interaction models
  - bond, angle, dihedral, improper styles = intra-molecular forces
  - kspace style = long-range interactions
  - fix style = added operations within a timestep
  - compute style = diagnostic calculations
  - region style = geometric regions
  - command style = new input script commands
  - dump style = flavors of per-atom output
  - min style = energy minimization algorithms

(5) Do you need help implementing the new feature ?

Find similar code already in LAMMPS

- Shows you which methods to define
- Shows you calls to make to other LAMMPS functionality
- Examples of functionality to find & mimic:
  - fixes that operate at same point in timestep
  - computes or fixes that need a neighbor list
  - computes or fixes that produce same kind of output data
  - fixes that persist per-atom data across timesteps
  - pair styles, fixes, computes that require communication

(5) Do you need help implementing the new feature ?

Find similar code already in LAMMPS

- Shows you which methods to define
- Shows you calls to make to other LAMMPS functionality
- Examples of functionality to find & mimic:
  - fixes that operate at same point in timestep
  - computes or fixes that need a neighbor list
  - computes or fixes that produce same kind of output data
  - fixes that persist per-atom data across timesteps
  - pair styles, fixes, computes that require communication

Ask the LAMMPS developers for advice

- Mail list, MatSci forum, create a GitHub issue
- Two reasons to not send email directly to the developers:
  - others can answer
  - Q and A is archived, so others can find it in the future

(6) Is this feature just for you or for public LAMMPS?

Just you: implement the feature however you want !

Public LAMMPS: follow guidelines on next slide

(6) Is this feature just for you or for public LAMMPS?

Just you: implement the feature however you want !

Public LAMMPS: follow guidelines on next slide

Why contribute your code to public LAMMPS ?

- Open source philosophy
- Fame and fortune
  - name on website author page and in source code
  - add a citation to your paper for LAMMPS to output
- People who use your new feature ...
  - find and fix bugs
  - extend its functionality
  - become collaborators

Rules of thumb for contributing code to LAMMPS

Next after next: Axel Kohlmeyer 45 min talk on this topic ...

- All code contributions are handled thru GitHub
  - fork or clone, create branch, submit a pull request
- See Submitting new features for inclusion in LAMMPS
  - section 3.2 of Programmer Guide
- Coding style in a one-line nutshell
  - write new code that looks like LAMMPS code
- Be sure to include:
  - doc page in RST format for each new command (doc/src)
  - if new model, new lammps/examples folder with input scripts
- Only create new style files
  - no non-trivial changes to LAMMPS core files
  - if you think it's unavoidable, ask developers first
- If unsure what is the LAMMPS way to do it, ask in advance
  - to avoid being asked to re-write your code

That's all

Questions?