How to modify LAMMPS

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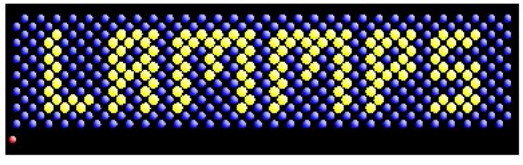

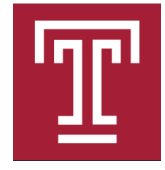

You have an idea for a new LAMMPS feature

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 ?

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First 4 Qs might convince you that you don't need to implement the feature within LAMMPS itself !

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- Maybe it can be incrementally extended
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Check the LAMMPS website and manual:

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

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

Two places to look:

- MatSci forum
  - new umbrella site for many materials modeling codes
  - MatSci forum link on LAMMPS webpage explains it
- GitHub issues
  - GitHub site: `https://github.com/lammps/lammps`
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If don't find anything, you can ask a Q on MatSci forum
Good to give big picture of what you want to do
May be already possible in ways you haven't thought about

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- Pre- or post-processing tasks $\Rightarrow$ website Pre/Post page
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  1. Invoke an external program from LAMMPS input script
     - could be an existing program or new program you write
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  2. Client/server coupling between LAMMPS and other code
     - data volume is modest: exchange by single procs
     - two independent codes, e.g. QM for AIMD or QM/MM
     - LAMMPS already has support for MDI coupling
     - can add MDI support to other code or wrap it with Python
     - see Section 8.8, Howto MDI in manual

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  3. Wrap an external library with new LAMMPS style
     - data volume is large: parallel exchange thru lib API
     - compute voronoi/atom wraps Voro++ lib for tesselation
     - pair_style kim wraps OpenKIM lib for potentials

Better done outside or inside LAMMPS ?

When the answer is generally inside:

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

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Many ways to use Python with LAMMPS:

- See section 2 of Programmer Guide
- Python script wraps LAMMPS as a library
  - invoke input script commands, query/set internal data
  - 3 interfaces: lammps.py, PyLammps, IPyLammps (Jupyter NBs)
  - fix external can call back to Python driver
- Use input script python variable ⇒ invoke Python function
  - Python function can call back to LAMMPS
- Fix python and pair_style python commands

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- Fix python and pair_style python commands
- Richard Berger gave 30 min talk on this at 2021 workshop
- Jan Janssen giving 1 hour breakout today on Pyiron

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Please take a look at the Programmer Guide
Axel has put lots of work into it over last 3 years
Being continuously improved – please suggest new content !

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Section 4: Information for Developers

- LAMMPS class hierarchy (fairly simple and flat)
- how a timestep works
- inter-processor communication options
- useful utility functions and classes
- low-level descriptions of LAMMPS internals
  - base classes
  - neighbor lists
  - parsing, file reading, Tokenizer class
  - distributed grids and FFTs

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- Modifying & extending LAMMPS - section 3 of Prog Guide
  - coding-oriented descriptions of all common styles
  - atom style = per-particle data
  - fix style = added operations within a timestep
  - compute style = diagnostic calculations
  - pair style = particle interaction models
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- Concrete examples for Writing new styles in section 4.8
  - step-by-step instructions with code snippets
  - 4 examples of a pair style, including a many-body potential
  - 1 example of a fix style
  - this is nice new content from Axel

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

Find a similar style 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 flavor of output data
  - fixes that persist per-atom data across timesteps
  - pair styles, fixes, computes that require communication

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Ask the LAMMPS developers for advice

- Via MatSci forum or create a GitHub issue
- Two reasons to not email the developers directly:
  - others can answer
  - Q and A is archived, so others can find it in the future
- Can send email to developers@lammps.org

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Just you: implement the feature however you want !

- you can even create an external package of related styles
- distribute it from your own website or your GitHub
- we can advertise your code: see External Packages on website

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Public LAMMPS: follow guidelines on next slide

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Why contribute your code to public LAMMPS ?

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

Rules of thumb for contributing code to LAMMPS

- All code contributions are handled thru GitHub
  - fork or clone, create branch, submit a pull request
- Read Submitting new features for inclusion in LAMMPS
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- Be sure to include:
  - doc pages in RST format for each new command (doc/src)
  - if new model, new lammps/examples folder with input scripts
- Limit your changes to 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
  - helps avoid being asked to re-write your code