Lecture #5b – Resources for LAMMPS info

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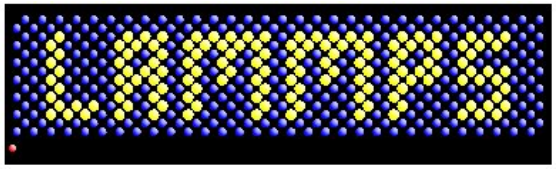
7th LAMMPS Workshop Tutorial
Virtual meeting – August 2021



Center for Computing Research

Sandia National Laboratories

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National Nuclear Security Administration

Goals for this 10 minute lecture

Show you how to ...

- Use the LAMMPS website and manual effectively
- Search for previous answers to Qs you have
- Find what others have done with LAMMPS

Go thru this first by slides ...
Will demonstrate in hands-on exercise

LAMMPS website: main menu at the top

https://www.lammps.org

- Download and GitHub: grab LAMMPS distro
- Manual: User Guide and Programmer Guide
- Commands: multiple alphabetized tables
  - doc page for every LAMMPS command
- Glossary: MD terms $\Rightarrow$ LAMMPS
- Workshops and Tutorials: past ones
- Publications: find papers related to your model
  - authors, titles, abstracts for 1000s of papers
  - browser search (e.g. Ctrl-F) for authors or title words
  - search abstracts (explained in a few slides)
- Pictures and Movies
  - user-contributed vignettes and paper links
- Pre/Post and External packages/tools
  - other software which works with LAMMPS
- Mail list and MatSci forum
  - how to ask Qs online and get or find answers

LAMMPS manual in two parts

Search bubble at top left of every page

- User Guide: also called the doc pages, 11 sections
  - Install, Build, Run, Accelerate performance
  - Commands and Packages
  - Howto discussions = 45 different topics
  - Tools = included in LAMMPS distribution
  - Individual doc pages for every LAMMPS command

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- Programmer Guide: 4 sections
  1. Library interface (C++, Fortran, Python)
  2. Using Python with LAMMPS - talk: Developers session
  3. Modifying & Extending - talk: Developers session
  4. Info for developers
     - class hierarchy
     - how a timestep works
     - coding details

Mail list and MatSci forum

See website Mail list and MatSci forum for full details

Mail list:

- Anyone can browse archive, ask Q, get answers to your Q
  - Qs from non-subscribers are moderated
- If subscribe, get emails for all messages
- Has archive of ∼80K messages over 15 years
  - more recent the message ⇒ the more helpful !

MatSci forum:

- Anyone can browse/search past Qs & As
- Must join forum to ask or answer Qs
- Mail list archive has been imported to forum
- MatSci has forums for many material modeling tools
  - discussions can cross-pollinate between tools

Three things to try with Google

1. Search the website
   - use Google search bar on home page
   - includes abstracts of papers on Publications page
   - try carbon nanotubes

Molecular dynamic simulation of defect-driven rotary system based ...
www.lammps.org › abstracts › abstract.17541.html
Molecular dynamic simulation of defect-driven rotary system based on a triple- walled **carbon nanotube** and graphene. XT Lin and Q Han, MOLECULAR

Simulation of static and dynamic mechanical characteristics of ...
www.lammps.org › abstracts › abstract.16518.html
The static and dynamic mechanical characteristics of **carbon nanotubes** with double and multiple vacancy defects are simulated by the molecular dynamics ...

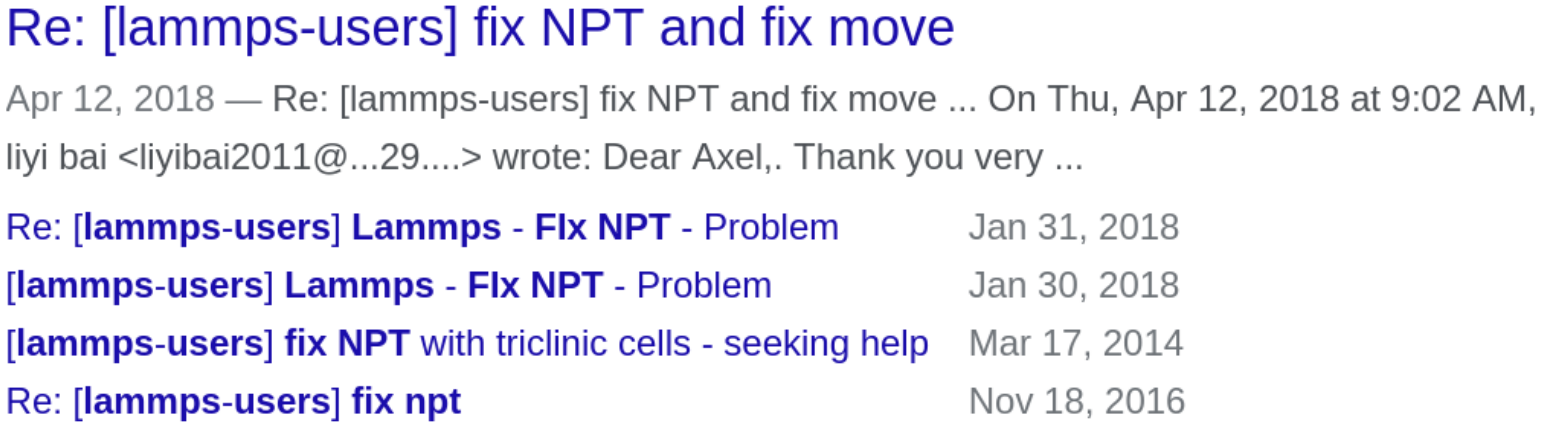
Interaction of Human Telomeric i-Motif DNA with Single-Walled ...
www.lammps.org › abstracts › abstract.17499.html
Interaction of Human Telomeric i-Motif DNA with Single-Walled **Carbon Nanotubes**: Insights from Molecular Dynamics Simulations. P Wolski and P Wojto
and K ...

Phononic thermal transport properties of C3N **nanotubes** MSR ...
www.lammps.org › abstracts › abstract.17840.html
It is found that the thermal conductivity of C3N nanotubes is significantly lower than those of **carbon nanotubes** across the entire ballistic-diffusive range.

Thermophoresis of Nanodroplets in Deformed **Carbon Nanotubes** ...
www.lammps.org › abstracts › abstract.17504.html
Carbon nanotubes based on mechanical deformation for controlling mass transport have various promising potential applications in nanofluidic devices.

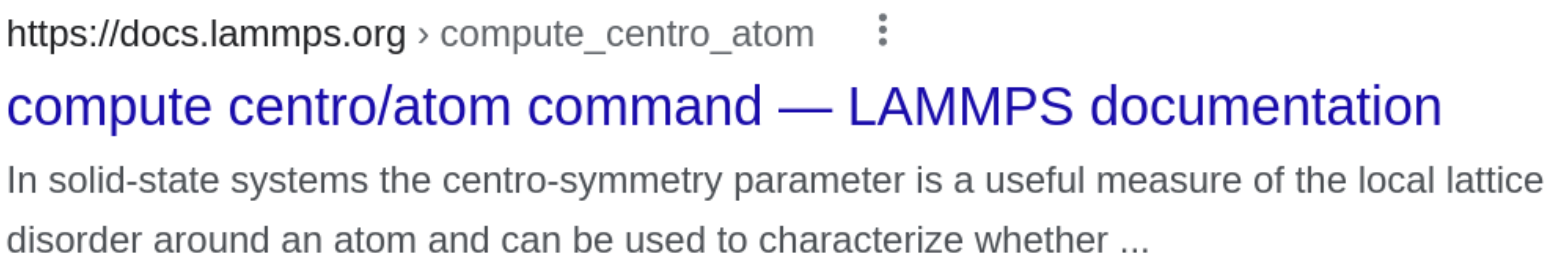
Three things to try with Google

2. Search the mail list archive
   - use Google search bar on Mail list page
   - or include lammps-users in regular Google search
   - try lammps-users fix npt



Three things to try with Google

3. Search for a sufficiently LAMMPS-specific term
   - try compute cna/atom



LAMMPS distribution has lots of input scripts

- 3 ways to grab the distro:
  - download tarball from website = current patch release
  - GitHub zip file = current master branch
  - GitHub clone repo = all versions of LAMMPS
- Examples dir: ~600 input scripts
  - lower-case dirs and PACKAGES = simple
  - upper-case dirs = more complex
  - many simple ones produce movies: see website Movies page

What have people already done with LAMMPS?

Model = description of system you want to simulate
Keywords = material, interatomic potential,
other unique attributes

- Search literature for model keywords + molecular dynamics
  - if another MD code has done it, maybe LAMMPS can also
- Search literature for model keywords + LAMMPS
  - maybe someone has done it with LAMMPS
- Search papers on website for authors or keywords
- Search mail list or forum for model keywords

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When all else fails ...

- Post a message to mail list or forum