LAMMPS User Workshop Albuquerque, NM 1 August 2017

LAMMPS Users' Workshop Beginner's Tutorial Download, build and run LAMMPS

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Getting started with LAMMPS

1. Explore resources and download

- Website
- File download

2. Make/build LAMMPS

- Downloading LAMMP
- Configuring for personal packages
- Building dependent libraries (FFT, JPEG, MPI, etc.)
- Building an executable for your architecture

3. Run LAMMPS

- Running a simple script
- Did it run? What did it do?

4. Where to learn more!



How to download, install, and use LAMMPS

Download page:

http://lammps.sandia.gov/download.html
Try the Windows serial executable – later.

Modify LAMMPS packages for your purposes:

make package_status make yes-shock make yes-reax make no-rigid make serial

• Installation instructions:

http://lammps.sandia.gov/doc/Section_start.html
go to lammps/src
type "make your_architecture"

To perform a simulation:

Imp –in *my script.in*



How to get help with LAMMPS

Excellent User's Manual:

http://lammps.sandia.gov/doc/Manual.html
http://lammps.sandia.gov/doc/Section_commands.html#3_5

- 2. Search the web: can include "lammps-users" as a search keyword to search user-group e-mail archives
- 3. Send e-mail to the user's e-mail list: http://lammps.sandia.gov/mail.html
- 4. Contact LAMMPS developers: http://lammps.sandia.gov/authors.html
 Steve Plimpton, siplimp@sandia.gov
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