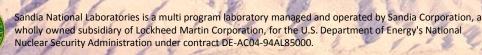
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2: Getting started with LAMMPS

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Overview

1. Explore our local tutorial network tools

- 1. Website
- 2. File upload/sharing

2. Start your virtual machines

- 1. Download and install VirtualBox
- 2. Download our tutorial ova file and start
- 3. Explore the workspace

3. Start LAMMPS

- 1. Downloading LAMMP
- 2. Configuring for rheology packages
- 3. Building an executable
- 4. Running a simple script
- 4. Practice w/ live demos for handling data and visualization
- 5. Where to learn more!



Local tools

- Local Network: http://192.168.1.10
- Course documents:
- LAMMPS Website snapshot:
- Web-based file sharing



How to download, install, and use VirtualBox

Download page:

https://www.virtualbox.org/wiki/Downloads

Installation and FAQ instructions:

https://www.virtualbox.org/wiki/End-user_documentation

To load the LAMMPS linux environment:

http://lammps.sandia.gov/LAMMPS Tutorial.ova

• Explore the major features:

Aurora web browser
Terminal window
Network and USB access
Save a system state



How to download, install, and use LAMMPS

Download page:

<u>lammps.sandia.gov/download.html</u>
Try the Windows serial executable – later.

Installation instructions:

<u>lammps.sandia.gov/doc/Section_start.html</u> go to lammps/src type "make your_system_type"

To perform a simulation:

lmp < my_script.in</pre>

Modify LAMMPS packages for rheology:

make package_status make yes-colloid make yes-rigid make serial

• To perform a simulation:

Imp < my script.in</pre>



How to download, install, and use VMD

Download page:

http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD

Installation instructions:

http://www.ks.uiuc.edu/Research/vmd/current/docs.html

Run and verify your rotating VMD:



Live demo #1: running a test example

- 1. Run example "obstacle"
 - /lammps/examples/obstacle
- 2. Modify the input script to produce JPEG output
 - Edit in.obstacle using vi or text editor
- 3. Use Image magic to view images and make movie



Live demo #2: visualizing output data

1. Plot the temperature from the log file

– gnuplot ...

2. Transfer your dump file to your native environment

- Use your browser to share files via website
- OR Use a thumb drive to share your file with your native environment

3. Visualize the simulation results using 3rd party software (VMD)

- Start up VMD and open the "atoms.lammpstrj" file
- View the "movie" you've made from the LAMMPS trajectory by pressing the play button.



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 old email archives
- 3. Try the wiki: http://lammps.wetpaint.com/
- 4. Send e-mail to the user's e-mail list:

http://lammps.sandia.gov/mail.html

5. Contact LAMMPS developers: http://lammps.sandia.gov/authors.html
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