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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 LAMMPS
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:**

lammps.sandia.gov/download.html

Try the Windows serial executable – later.

- **Installation instructions:**

lammps.sandia.gov/doc/Section_start.html

go to lammps/src

type “*make your_system_type*”

- **To perform a simulation:**

`Imp < my_script.in`

- **Modify LAMMPS packages for rheology:**

`make package_status`

`make yes-colloid`

`make yes-rigid`

`make serial`

- **To perform a simulation:**

`Imp < my_script.in`

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”

- `/lammers/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

1. Excellent User's Manual:

<http://lammeps.sandia.gov/doc/Manual.html>

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

2. Search the web: can include “lammeps-users” as a search keyword to search old e-mail archives

3. Try the wiki: <http://lammeps.wetpaint.com/>

4. Send e-mail to the user's e-mail list:

<http://lammeps.sandia.gov/mail.html>

5. Contact LAMMPS developers: <http://lammeps.sandia.gov/authors.html>

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