Getting Started with LAMMPS

Connect to the local LAMMPS Intranet:

Start your machine's wireless and connect to the network:

SSID: LAMMPS (Open, No passcode required)

Open your browser and type the following address:

http://10.1.1.10 (the address is all numbers).

Have a look at the LAMMPS website:

You will be using this a LOT over the next two days.

Find the Manual and have a look at the commands. Bookmark this page.

Test the file transfer capability:

Your username is your last name in lower case.

Your password is the first three letters of your first name (lower case).

You can change your password.

Upload a small file or image from your local machine. THIS WILL BE PUBLIC!

VirtualBox Software:

Open Oracle VirtualBox

Select FILE -> Import Appliance

Click "Open Appliance…" and select LAMMPS_Tutorial14.ova which you had previously downloaded.

Click "Import"

The LAMMPS_Tutorial14 appliance should appear on the left with the identifier "Powered Off."

IMPORTANT NOTE: You only need to Import the Appliance once. If you do this more than once you will create multiple complete instances of the Virtual Machine on your computer. Do not double-click on the ova icon to open an appliance.

Configure the LAMMPS_Tutorial appliance for your host environment.

Select "Settings" under the gear icon in the Oracle VM VirtualBox Manager.

For most users only the "Network" will need to be altered. To do this, select the network icon on the top and select Adapter 1. "Enable Network Adapter" should already be checked. Confirm that you are already attached to "Bridged Adapter."

Change the "Name" of the adapter by selecting your wireless adapter from the pull-down menu.

Leave all the "Advanced" settings unchanged.

Click OK. You are ready to start the appliance.

Now start the LAMMPS_Tutorial14 appliance by selecting it and clicking the green arrow labeled "Start."

You will receive several warnings as the machine starts up.

Keyboard capture: When the window is selected the keyboard entry will go to the virtual machine. Disable the warning.

Mouse Integration: Most machines aren't good at this. So we'll turn it off as soon as the machine is started. Disable the warning.

Congratulations! You are running a lightweight version of Linux on your computer! And, LAMMPS is already installed.

Setup your Linux environment:

Explore the application dock at the bottom of the screen.

Select the "Control Panel" (fourth from the left)

Click "Date/Time" and set the system time.

Click "Network" and near the top simply click "yes" under "Use DHCP Broadcast?" Then "Apply." Then "Exit." And, close the control panel.

Test the network connectivity by opening "Arora_browser" (right-most icon).

The browser should open to the LAMMPS Intranet http://10.1.1.10.

Download the file that you uploaded from your host OS.

Open a "Terminal" window (second from the left).

This will be your main tool to explore the virtual environment.

Pick-up a hand-out on Unix/Linux commands and vi Editor.

IMPORTANT NOTE: There is no "undo" in any of tools in TinyCore Linux. This means not even a back button in the browser. Beware!

Setup and explore your LAMMPS setup:

Open "Terminal" And type "`ls`" to get a directory listing. Try "`ls –al`" to get more file information.

Change directory to lammps with "`cd lammps`"

Feel free to continue to explore with ls and cd.

Now let's go to where the action happens, which is ~/lammps/src. This is the source code of lammps and where the executable is configured and made using a unix/linux command called "make"

To see how you can configure LAMMPS type: `make help`

To see all the packages that are loaded type: `make package-status`

To add the package colloid type: `make yes-colloid`

To add the package misc type: `make yes-misc`

Were the two packages added? To check type: `make package-status`

When you are done type: `make serial`

That last command did the work to compile the code and create an executable. The machine type "serial" refers to the fact that this build is designed to run on only one processor. The machine type is always appended to the executable name. In this case, lmp_serial

Test LAMMPS on the obstacle example:

In a Terminal window, move to ~/lammps/examples/obstacle. Check the contents with "`ls –al`"

To test that LAMMPS is setup. Type "`lmp_serial < in.obstacle`"

You should get some output to the screen and a log file "log.lammps".

Now edit the file "in.obstacle" to remove the comments (# beginning the lines) around the dump lines at the end. Rerun "`lmp_serial < in.obstacle`" and see that there is additional output produced by the dump commands with "`ls –al`"

View one of the visual dump files "`display image.18000.jpg`"

Now string them all together "`convert image*.jpg movie.gif`"

Display in the browser with "`arora movie.gif`"

Move your dump file from the obstacle example and view in VMD:

With arora still open, go back to the LAMMPS Intranet. Log into your upload area and upload the dump file you just created
(i.e. ~/lammps/examples/obstacle/dump.obstacle)

Minimize your virtual machine and move back into your HOST ENVIRONMENT

Open a browser in your HOST ENVIRONMENT and go to the Intranet. Download your dump.obstacle file from your fileshare directory. This is the only way to move data from your virtual machine to your host machine.

Open VMD and in "VMD Main" Select File -> New Molecule

Browse to the file you just pulled down from the intranet.

Under Determine file type: select "LAMMPS trajectory" and Click "Load"

In the window "Graphical Representations" select Drawing Method "VDW" from the pull-down. Then use your mouse to rotate and zoom the 3D representation. Use the arrows below the image to play through the trajectory. **Congratulations! You are ready for the hands-on activities…**