Basic LAMMPS builds

Have a look at the LAMMPS website: <u>http://lammps.sandia.gov</u> Bookmark this page. WINDOWS INSTALL

Determine whether you are running 32-bit or 64-bit Windows

Click Start, then right click on "Computer" and select "Properties"

From the main LAMMPS Downloads page select Windows Installer (near bottom) and choose the appropriate version for your system and "Save" or "Save As"

When the download completes, double-click to launch the installer and select "Run". You will be warned of an "Unknown Publisher". The launcher will unpack the LAMMPS directories into your Program Files directory and add the directory to your path.

MACINTOSH INSTALL

Make sure that you have Xcode installed on your mac by typing "gcc" at a command prompt. If you don't have Xcode, then you will be prompted to install.

Follow the Linux Install instructions from there.

LINUX INSTALL

From the main LAMMPS Downloads page select "LAMMPS --- Stable version" and then "Download Now"

When the download completes, go to the directory containing the file and type "tar —xvf lammps-15May15.tar" This will unpack the LAMMPS directories.

Type "cd lammps-15May15/src". Feel free to continue to explore with ls and cd. This is the source code of lammps and where the executable is configured and made using a unix/linux command called "make"

Type: make mpi-stubs Thentype: make -j8 serial

That last command did the work to compile the code and create an executable. This might take a while to complete. The machine type "serial" refers to the fact that this build is designed to run on only one processor and with the internal fft solver. When complete, the executable will lmp_<machine>, in this case lmp_serial

Test LAMMPS on the obstacle example:

LINUX/MAC: In a Terminal window, move to ~/lammps/examples/obstacle. Test that LAMMPS is setup. Type "../../src/lmp_serial < in.obstacle" You should get some output to the screen and a log file "log.lammps".

Windows: Open a "Command Prompt" window and type "cd "\Program Files\LAMMPS XX-bit 20150724\Examples\obstacles"", where XX is either 32 or 64 bit.

Type "lmp_serial <in.obstacle" to launch LAMMPS with the input script.

Congratulations! You are ready for the hands-on activities...