1.021, 3.021, 10.333, 22.00 Introduction to Modeling and Simulation
Spring 2018

Recitation #3

Linux/Unix, LAMMPS, and application to FCC Cu crystal deformation.

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Massachusetts Institute of Technology

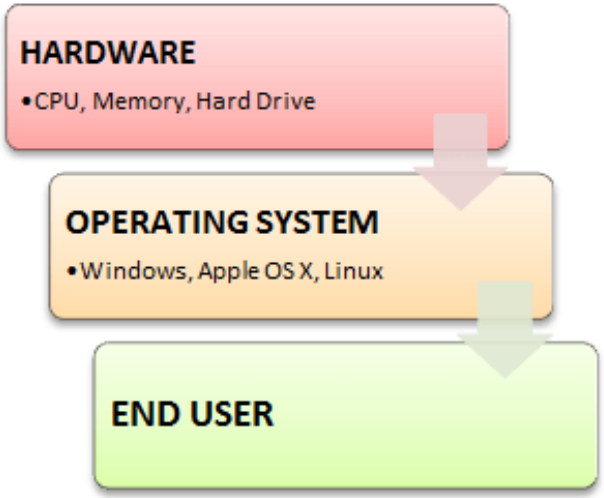
Review from last week

- Any comments/changes on working groups for Psets?
- Questions?

Basics on Unix/Linux

What is UNIX?

UNIX is an **operating system** which was first developed in the 1960s. It is stable, multi-user, multi-tasking system for servers, desktops and laptops.



Types of UNIX

There are many different versions of UNIX: Sun Solaris, **GNU/Linux**, and **MacOS X**.

The UNIX operating system

The kernel of UNIX is the hub of the operating system. It allocates time and memory to programs.

The shell acts as an interface between the user and the kernel.

What is GNU/LINUX?

GNU/Linux is UNIX-like operating system (Linux Kernel + GNU tools). The Linux kernel was released by **Linus Torvalds** as free, *open-source* software in 1991. The code is fully visible, and can be modified and redistributed.

"Types" of LINUX (distributions)

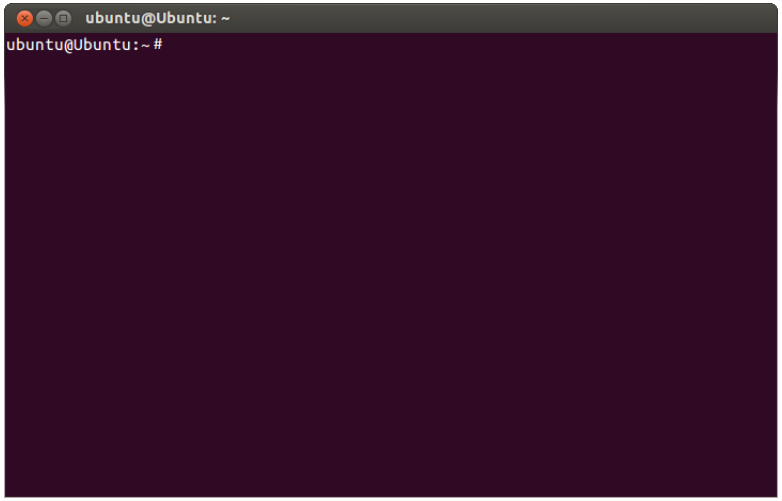
There are more of 300 LINUX distributions. Some common examples are:

- Debian-based Linux distributions (.deb packages): Debian, **Ubuntu**
- RPM-based distributions (RedHat, Fedora, OpenSuse)
- Others: Gentoo

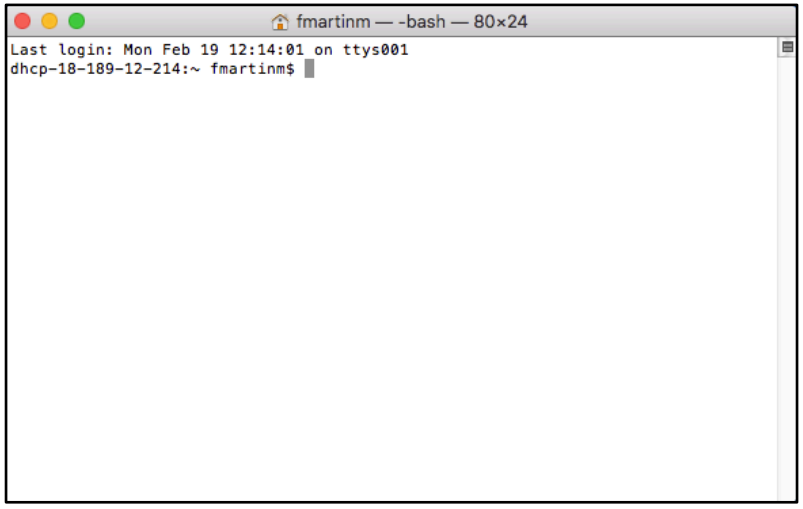
The LINUX operating system

Strictly speaking, Linux is the *kernel*, not the entire operating system. The rest of the operating system usually includes many GNU libraries, utilities, and other software, from the Free Software Foundation. The operating system as a whole is known as GNU/Linux

Ubuntu (Terminal)



MacOS (iTerm)



Windows 10 - Use “PuTTY” for remote access or:

Using LAMMPS with Bash on Windows

written by Richard Berger

Starting with Windows 10 you can install Linux tools directly in Windows. This allows you to compile LAMMPS following the same procedure as on a real Ubuntu Linux installation. Software can be easily installed using the package manager via apt-get and all files are accessible in both the Windows Explorer and your Linux shell (bash). This avoids switching to a different operating system or installing a virtual machine. Everything runs on Windows.

http://lammps.sandia.gov/doc/tutorial_bash_on_windows.html

Basic Commands

- ls
  - $ ls -l
  - $ ls -a
  - $ ls -la
  - $ ls -l --sort=time
  - $ ls -l --sort=size -r
- cd
  - $ cd /usr/bin
- pwd
  - $ pwd
- ~
  - $ cd ~
- ~*user*
  - $ cd ~fmartinm

- What will “cd ~/fmartinm” do?

- which
  - $ which ls
- whereis
  - $ whereis ls
- locate
  - $ locate file.txt
- find
  - $ find / | grep stdio.h
  - $ find /usr/include | grep stdio.h

Basic Commands (cont)

- cat
  - $ cat /etc/motd
  - $ cat /proc/cpuinfo
- cp
  - $ cp foo bar
  - $ cp -a foo bar
- mv
  - $ mv foo bar
- mkdir
  - $ mkdir foo
- rm
  - $ rm foo
  - $ rm -rf foo
  - $ rm -i foo
  - $ rm -- -foo
- chgrp
  - $ chgrp bar /home/foo
- chown
  - $ chown -R foo:bar /home/foo
- chmod
  - $chmod a+x /home/foo/file.sh

Basic Commands (cont)

- tar
  - $ tar cvfp lab1.tar lab1
- gzip
  - $ gzip -9 lab1.tar
- untar & ungzip
  - $ gzip -cd lab1.tar.gz | tar xvf –
  - $ tar xvfz lab1.tar.gz

Connecting remotely

$ ssh fmartinm@sunray2.mit.edu

Vim – vi file.ext

- 2 modes
  - Input mode
    - ESC to back to cmd mode
  - Command mode
    - Cursor movement
      - h (left), j (down), k (up), l (right)
      - ^f (page down)
      - ^b (page up)
      - ^ (first char.)
      - $ (last char.)
      - G (bottom page)
      - :1 (goto first line)
    - Swtch to input mode
      - a (append)
      - i (insert)
      - o (insert line after
      - O (insert line before)
- Delete
  - dd (delete a line)
  - d10d (delete 10 lines)
  - d$ (delete till end of line)
  - dG (delete till end of file)
  - x (current char.)
- Paste
  - p (paste after)
  - P (paste before)
- Undo
  - u
- Search
  - /
- Save/Quit
  - :w (write)
  - :q (quit)
  - :wq (write and quit)
  - :q! (give up changes)

Emacs – emacs file.ext

- $ emacs
- Cursor movement
  - ^f (forward one char.)
  - ^b (backward one char.)
  - ^a (begin of line)
  - ^e (end of line)
  - ^n (next line)
  - ^p (prev. line)
  - ^v (page up)
  - alt-v (page down)
- Deletion
  - ^d (delete one char)
  - alt-d (delete one word)
  - ^k (delete line)
- Paste
  - ^y (yank)
- Undo
  - ^/
- Load file
  - ^x^f
- Cancel
  - ^g
- Save/Quit
  - ^x^c (quit w/out saving)
  - ^x^s (save)
  - ^x^w (write to a new file)

Basics on LAMMPS

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

Download LAMMPS

There are several ways to get the LAMMPS software.

- **Source tarball:** You can follow the download instructions on this page to grab a source tarball, and then follow the instructions in Section Getting Started of the LAMMPS manual to use "make" and build an executable for any machine.
- **Git or SVN:** If you have Git or Subversion (SVN) installed on your machine, you can use checkout and update commands to get the LAMMPS files once and then stay current. You then build LAMMPS from source as you would with the tarball. Both Git and SVN access is provided by GitHub. Further instructions for Git and SVN access are below.
- **Pre-built Linux executables:** For Ubuntu it is a personal package archive (PPA). For Fedora/RedHat/CentOS/openSUSE it is a binary RPM. The executable includes all LAMMPS packages that do not use additional libraries from the lib directory (e.g. MEAM, GPU, etc) and is kept up-to-date daily. Further instructions on this are below for Ubuntu and RPMs.
- **Automated Mac build:** OS X users can use the popular package manager Homebrew to download, build, and install LAMMPS, the Python module, and additional files and resources (i.e. potential files, tools, etc). Further instructions on this are below for OS X with Homebrew.
- **Pre-built Windows executables:** Windows users can download an installer package from this site. Installers for different dated versions of LAMMPS are available, either as 32-bit and 64-bit variants. The most current installer package is updated several times per month, more often than the "stable" version listed below as a source download. The installer doc page also describes how to run the executables in serial or parallel, using MPICH (which you must also install). More details are described below in the Windows installer section.

- Download a tarball
- Git checkout and update
- SVN checkout and update
- Pre-built Ubuntu executables
- Pre-built binary RPMs for Fedora/RedHat/CentOS/openSUSE
- Pre-built Gentoo executable
- OS X with Homebrew
- Windows installer package
- Applying patches

Building LAMMPs yourself (Compiling):

http://lammps.sandia.gov/doc/Section_start.html#making-lammps

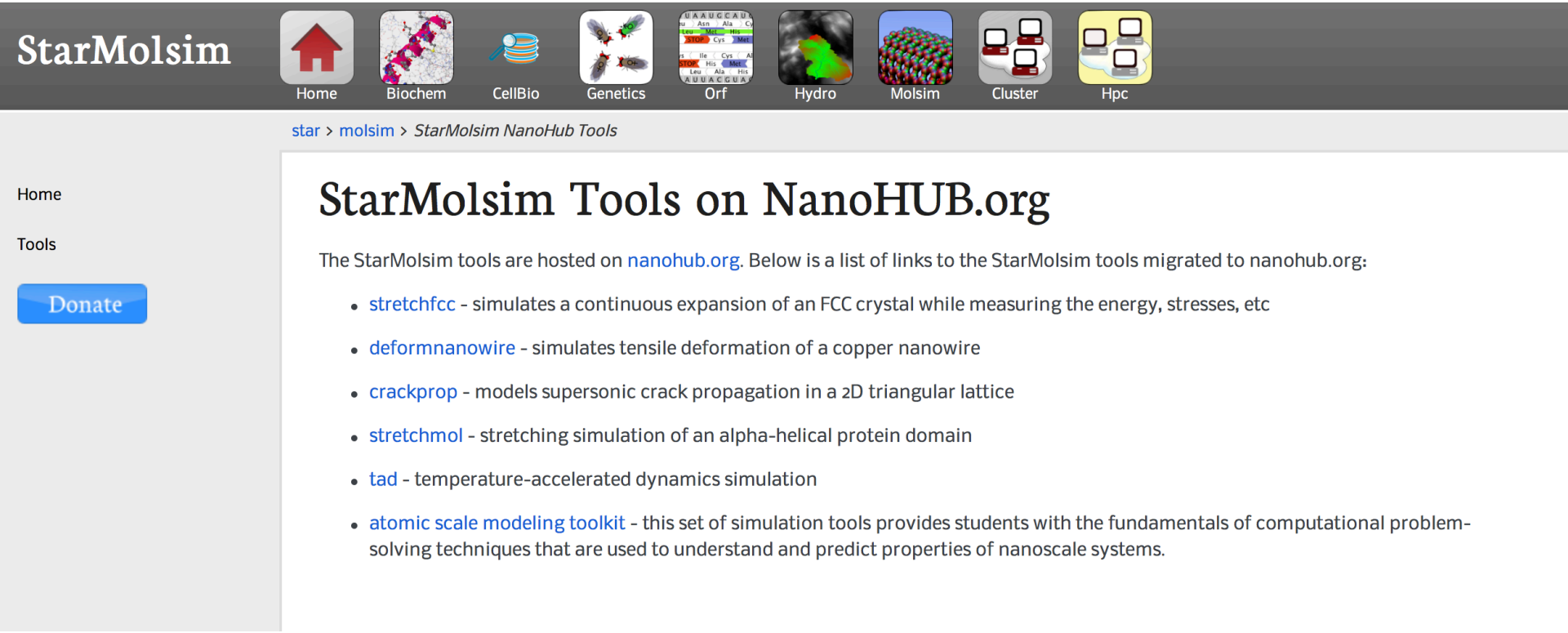
For windows:

http://rpm.lammps.org/windows.html

http://lammps.sandia.gov/doc/tutorial_bash_on_windows.html

LAMMPS using nanoHUB

Simulation index (MIT tools for IM/S): http://star.mit.edu/molsim/nanohub/index.html



Collect

Stretching Simulation of FCC Crystal

By Markus Buehler[1], Justin Riley[1], Joo-Hyoung Lee, Jeffrey C Grossman[2]

1. Massachusetts Institute of Technology (MIT) 2. Massachusetts Institute of Technology

This tool simulates a continuous expansion of an FCC crystal while measuring the energy, stresses, etc

Launch Tool

Version 1.2 - published on 03 Sep 2014

doi:10.4231/D35717P48 cite this

View All Supporting Documents

Tool Audience Unrated

262 users, detailed usage

0 Citation(s)

1 question (Ask a question)

0 review(s) (Review this)

0 wish(es) (New Wish)

Share: ...

Watch resource

When watching a resource, you will be notified of changes made. You may stop watching at any time.

Category

Tools

Published on

03 Sep 2014

Crystal Geometry | Lennard-Jones Parameters | Strain Increments | Boundary Conditions | Simulation Parameters

Lattice Constant: 3.615

Unit cells in x-direction: 4

Unit cells in y-direction: 4

Unit cells in z-direction: 4

Run Experiment »

Stretching Simulation of FCC Crystal (2:54 pm) | Terminate | Keep for later

Stretch FCC Crystal | Jmol ×

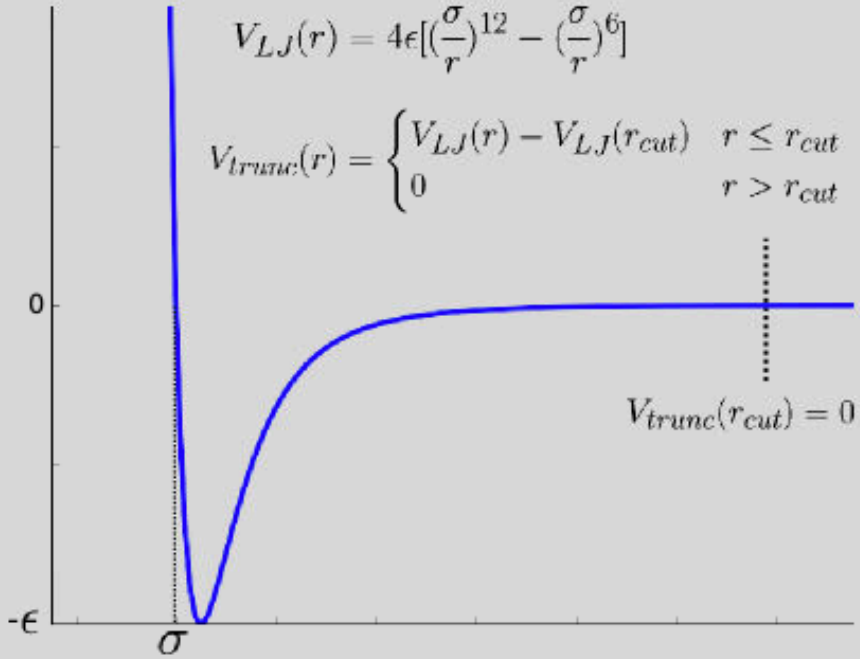
1 Input → 2 Run Experiment

Crystal Geometry | Lennard-Jones Parameters | Strain Increments | Boundary Conditions | Simulation Parameters

Cutoff of potential: **5.38**

Epsilon: **0.204**

Sigma: **2.616**



Run Experiment »

Storage (manage) 9% of 10GB

857 x 585

Stretching Simulation of FCC Crystal (2:54 pm) | Terminate | Keep for later

Stretch FCC Crystal | Jmol ×

1 Input → 2 Run Experiment

Crystal Geometry | Lennard-Jones Parameters | Strain Increments | Boundary Conditions | Simulation Parameters

Strain increment interval: 100

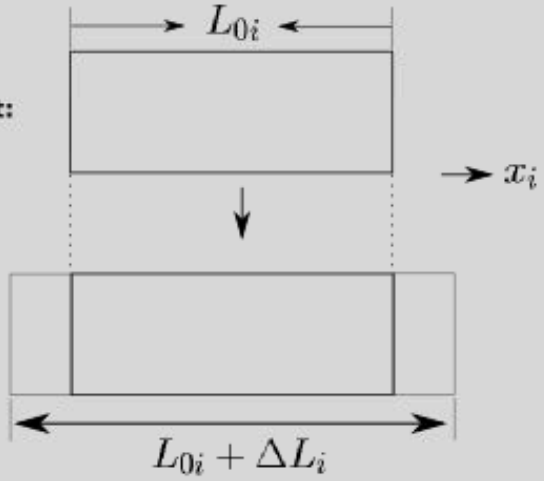
Strain increments in the X direction: 0.01

Strain increments in the Y direction: 0.01

Strain increments in the Z direction: 0.00

Strain Increment:

$$\epsilon = \frac{\Delta L_i}{L_{0i}}$$



Run Experiment »

Storage (manage) 9% of 10GB

857 x 585

Crystal Geometry | Lennard-Jones Parameters | Strain Increments | Boundary Conditions | Simulation Parameters

periodic boundary conditions in X: yes

periodic boundary conditions in Y: yes

periodic boundary conditions in Z: yes

Run Experiment >

Stretching Simulation of FCC Crystal (2:54 pm) Terminate Keep for later

Stretch FCC Crystal | Jmol

1 Input → 2 Run Experiment

Crystal Geometry | Lennard-Jones Parameters | Strain Increments | Boundary Conditions | Simulation Parameters

From previous recitations…

What are the units of the timestep?

And the units of Temperature?

Starting temperature:	0.0000000000001
Maximum number of steps:	8000
Time step:	0.25
How often is energy and stress information written:	5
How often is check-point information written:	100

Run Experiment »

Storage (manage) 9% of 10GB 857 x 585

Result: Input File

- Initial Crystal (XYZ)
- Stress vs Simulation Step
- Output Data
- Input File
- Simulation Movie (XYZ)
- Output Log
- ---
- Download

```
# Box
box_x
box_y
box_z


#PARAM
pbc_di
lindef_interval   100          # number of steps between linear deformation
lindef_size       1.                        # size of linear deformation
lindef_x          0.01 0.  0.       # first row vector of the deformation matrix
lindef_y          0.   0.01 0.      # second row vector of the deformation matrix
lindef_z          0.   0.   0.01    # third row vector of the deformation matrix (only

#PARAMETER:  the following three lines as before...
eng_int         5
checkpt_int     100
press_int       1000000

starttemp       1e-13

seed            308989
```

Find: Select All

1 result Clear

< Input

Input coordinates

Steps

Timestep

Cutoff

LJ parameters

Unit cell

Deformation

```
simulation      1

coordname       crystal.xyz
outfiles        OutFile1001  #

ensemble        nve
startstep       1
maxsteps        8000

timestep        0.25

total_types     3
ntypes          1

#core_potential_file    cu_pair.dat
#embedding_energy_file  cu_emb.dat
#atomic_e-density_file  cu_den.dat

r_cut    5.38 # between 3rd and 4th nearest neighbor
#r_cut   3.4  # nearest neighbor (your own LJ potential)
r_begin  0.4
pot_res  1000

lj_epsilon      0.204
lj_sigma 2.616  # CLERI

# Box size (copy from el110 run)
box_x   20.449528 0.00 0.00
box_y   0.00 20.449528 0.00
box_z   0.00 0.00 14.460000


#PARAMETER (PBCs, as before...)
pbc_dirs        1 1 1

lindef_interval   100       # number of steps between linear deformation
lindef_size       1.                        # size of linear deformation
lindef_x          0.01 0. 0.       # first row vector of the deformation matrix
lindef_y          0.  0.01 0.      # second row vector of the deformation matrix
lindef_z          0.  0.  0.0     # third row vector of the deformation matrix (onl

#PARAMETER:  the following three lines as before...
eng_int         5
checkpt_int     100
press_int       1000000

starttemp       1e-13

seed            308989
```

How would it looks if you want to run it in LAMMPS?

Analyze the change in stress in different directions.

What happens if we increase the timestep?

Run it!