MD-Primer
LAMMPS

Stefan Bringuier

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Molecular Dynamics Primer: LAMMPS Examples

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LAMMPS

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LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.

Adapted from lammps.sandia.gov

Design of LAMMPS

License

- LAMMPS is provided through GNU Public License

- Free to use, modify, and distribute

Code Layout

- Object-Oriented approach

- Parallelization via Message Passage Interface (MPI)

- Is invoked by commands through input scripts
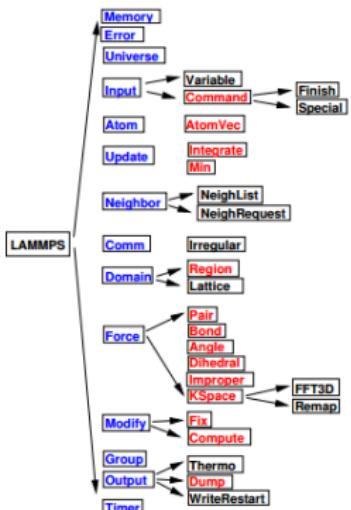
Figure 1: Class hierarchy within LAMMPS source code.

Adapted from lammps.sandia.gov

Obtaining LAMMPS

Download Source

Point your browser to lammps.sandia.gov/download and download the tarball. This allows you to compile LAMMPS to your liking!

Preferred Method For Beginners

Many hard working people have set up repositories for linux/unix binaries as well as windows executables. Go to lammps.sandia.gov/download and find the appropriate link for *Pre-built* executables.

LAMMPS performance

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Resource Usage

- Typically script prototyping and trouble shooting is done on user desktops and laptops.
- Actual MD simulations usually require significant resources
- High Performance Computing services
- Group computing server (12-36 cores)

Scaling

Adapted from lammps.sandia.gov
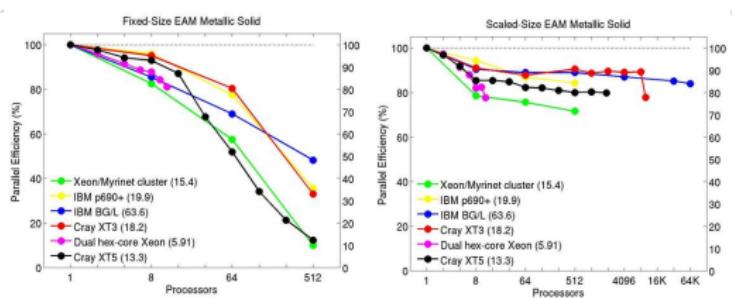
HPC at UofA

Getting an Account

Request for a user account requires a sponsor, namely, your advisor. Each sponsor is given 10,000 CPU hours of *standard* allocation.

Visit http://rc.arizona.edu for more details.

Real Quick: Running LAMMPS on HPC

```
#Load lammps binary
module load lammps/3feb13

#serial
lmp -l log.file -in in.file

#parallel
mpirun -np num_procs lmp -l log.file -in in.file
```

Resources

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Use the Manual!

- The LAMMPS manual has almost all your questions answered.
- Manual:
  http://lammps.sandia.gov/doc/Manual.html
- Search the mailing list:
  http://lammps.sandia.gov/mail.html
- Subscribe and Email the mailing list (https://lists.sourceforge.net/lists/listinfo/lammps-users)

Adapted from www.martybucella.com

Continued...

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Visualization Tools and Builders

- Checkout
  http://lammps.sandia.gov/prepost.html
- OVITO http://www.ovito.org
- VMD, http://www.ks.uiuc.edu/Research/vmd

Adapted from http://www.ovito.org
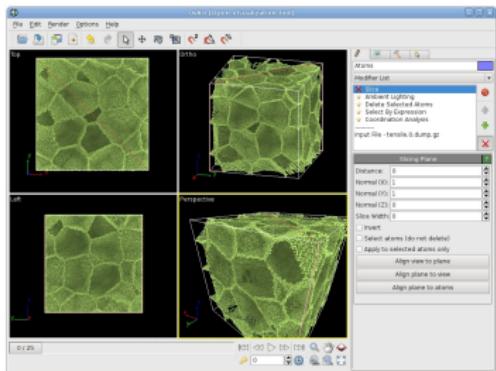
Outline of LAMMPS Input script

Command Line Driven

LAMMPS has no standard GUI. Every simulation is executed by supplying an input text script to the LAMMPS executable.

Parts of An Input Script

- Initialize: units, dimensions, etc.
- Atomic positions and velocities
- Settings:
  - Interatomic potential
  - Run time simulation parameters (e.g. timestep)
  - Fixes - operations during dynamics (e.g. thermostat)
  - Computes - calculation of properties during dynamics
- Run!

Example 1: Energy vs. Volume

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Example 1: BCC Iron
This is more of a static calculation however we can get some useful material properties.

Listing 1: Simulation Settings

```
# Energy:eV  Distance:Angstrom  Mass:Kg  Time:picosec
units       metal

#Classical particles
atom_style   atomic

#p=Periodic, in x y z
boundary     p p p
```

Continued...

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Listing 2: Specify The Structure

```
#lattice constant i.e. Fe-BCC 2.8665
variable a equal 2.8665

# BCC structure
lattice bcc $a

# Specify simulation box
region box block 0 5 0 5 0 5

# Initiate box with 1 atom type
create_box 1 box

# Create 1 atom type on lattice in simulation box
create_atoms 1 box

mass 1 55.85
```

Continued...

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Listing 3: Interatomic Potential

```
# Interatomic potential — Embedded Atom Method
pair_style eam/fs

# interaction pairs, filename, Element parameters
pair_coeff * * Fe_mm.eam.fs Fe

#Specify build neighborlist, use cutoff+0.3 A
neighbor   0.3 bin

#Frequency to rebuild neighborlist
neigh_modify every 20 delay 0 check no
```

Continued...

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Listing 4: Output Configuration

```
#Compute the energy per atom
compute eperat all pe/atom

#Output x,y,z of atoms LAMMPS standard format
dump config all atom 10 dump.FeBCC_${a}

#Custom output of atom properties
dump config all custom 10 dump.FeBCC_${a} &
 id type x y z c_eperat
```

Listing 5: Dynamics

```
timestep 0.001

#Ensemble
fix 1 all nve

#Frequency of Ensemble data output to screen
thermo 500

#Data that is output to screen
thermo_style custom step pe ke temp vol press
run 10000
```

Results of Example 1

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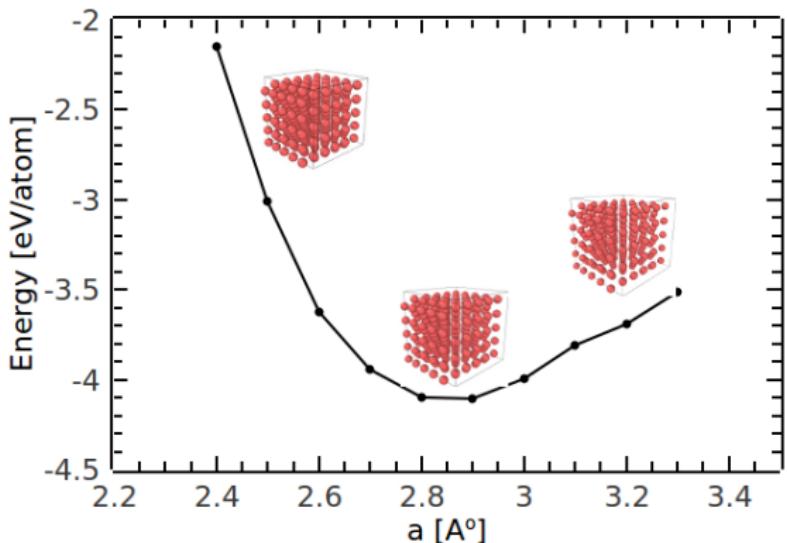
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Figure: Fe-BCC Energy vs. lattice parameter. Experimental lattice parameter, a=2.865

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Elastic Constants

Not show in the input script of example 1 but we can obtain the static elastic constants with fair ease.

C_{11}	244 GPa
C_{12}	145 GPa
C_{44}	116 GPa

Table: Elastic constants for BCC Fe

Example 2: Melting Nanoparticle

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Example 2: Attempt to observe melting of gold nanoparticle
Many of the commands for this example are similiar to the
example 1. The nanoparticle was created by using the
"region" command.
Potential - EAM for gold

Listing 6: RDF & minimize

```
# Get the radial distribution function
compute rdf all rdf 50
fix rdf1 all ave/time 100 10 1000 c_rdf &
 ave running file nanogold.rdf mode vector

#Energy & Force tolerence ,max iterations.
minimize 1.0e-8 1.0e-8 1000 100000

#Minimize using conjugate gradient method
min_style cg
```

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Listing 7: NVT-Melt

```
timestep 0.001

#Frequency of Ensemble data output to screen
thermo 5000
thermo_style custom step pe ke etotal temp vol press

#Thermalize to 298 K
#Create velocity distribution
velocity all create 298 39849 &
 mom yes rot yes dist gaussian

# NVT ensemble ramp temperature to melt
fix             2 all nvt temp 298.00 2400.00 1.0
run  100000
```

Results for Example 2

Watch it Melt!

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Further Confirmation
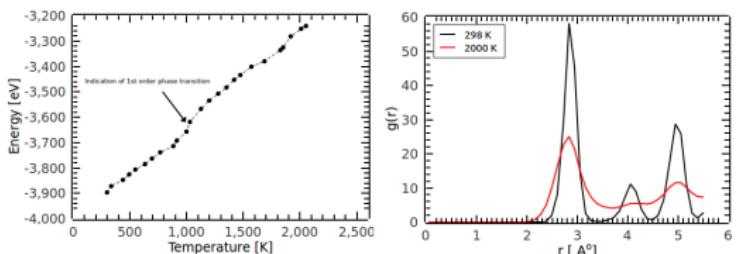
Figure: (a)Au nanoparticle melting (b) Radial distribution function

Things to Try!

- Change the diameter of the nanoparticle, what happens?
- Does the melting temperature change?
- What about a nanoparticle with different facets?
- Could we crystallize nanoparticles from a melt?

Example 3: Sputtering

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Example 3: This is a more advanced simulation (NEMD)
which looks at the sputtering of carbon onto (100) Si.
Like examples 1 and 2 many of the basic commands are the
same only a few other commands are added
Potential - Tersoff 1989 version

Listing 8: Regions & Sputter

```
# p = periodic , f= fixed
boundary        p p f
...
...
# Set the force on atoms in bottom to Zero
fix s1 fbot setforce 0.0 0.0 0.0
...
...
#Basic setup sputtering of carbon on Silicon.
fix 4 all deposit 500 2 500 95485 region sput near 1.2 &
vz −0.5 −1.5 target 12.0 12.0 28.0 units box
```

Results

Let it Rain!

Things To Try!

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- What happens when you do this at higher temperatures?
- What is the effect of sputtering rate?
- How can we quantitatively measure thickness?
- Is exposed surface important?

Questions?

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Please feel free to contact me to setup a 1-on-1 session if you have specific questions or need help running LAMMPS on your system(s).

If you would like to obtain a copy of this presentation you can email me at *stefanb@email.arizona.edu*