24-623: LAMMPS Lecture 3/8/2011

Outline

- LAMMPS Overview
- LAMMPS Installation
- LAMMPS Example How to Run
- LAMMPS Example Code
- LAMMPS Example Results
- LAMMPS Performance
- LAMMPS Modifications
- LAMMPS Post-Processing
- Discussion

LAMMPS Overview

- LAMMPS = “Large-scale Atomic/Molecular Massively Parallel Simulator”

http://lammps.sandia.gov/

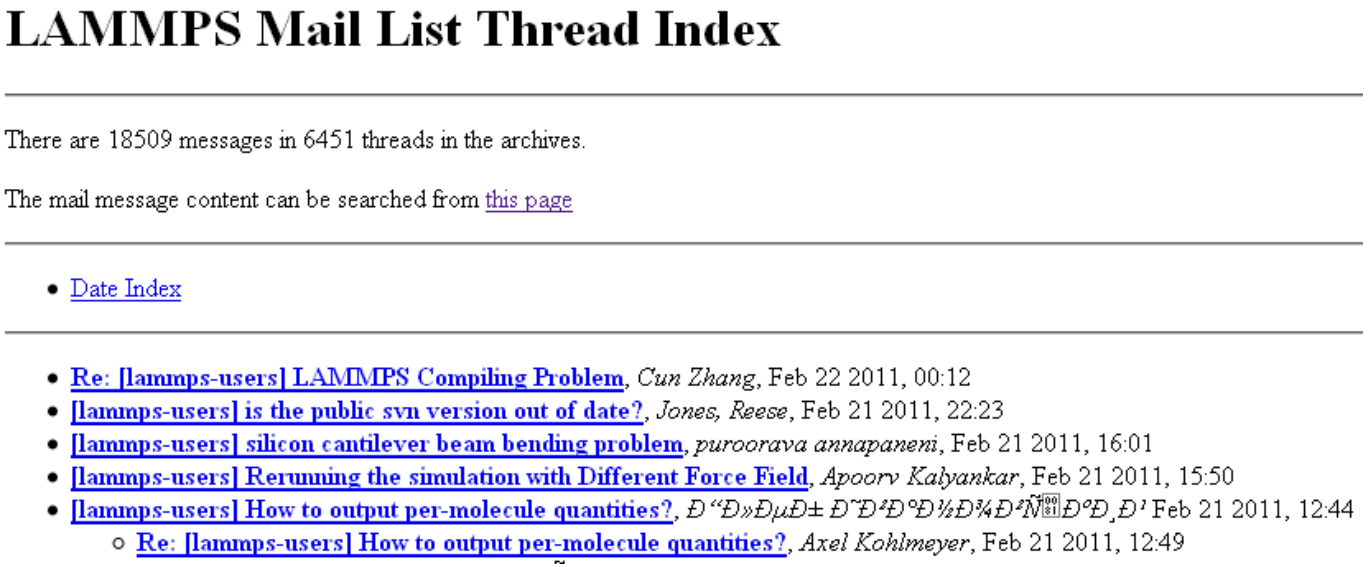
FEATURES:

- **LAMMPS has many potentials**, including potentials for biological systems, colloids, granular materials, metals, etc.
- **LAMMPS has many built in functions** (computes) that can automatically calculate/average quantities (Temp., Press., MSD of atoms, RDF, thermal conductivity, etc.).
- **LAMMPS is an open source code** in C++. Anyone can modify the code. Older versions in F90/F77 are available as well as Windows version.
- **LAMMPS is a parallel code**. It can be run on single cpu or in parallel using MPI and spatial-decomposition of simulation domain.

LAMMPS Overview: Support

- LAMMPS has an excellent mailing list that began in 2005 and has >10,000 messages. Probably the best discussion forum I've seen of all open source simulation codes.

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



LAMMPS Mail List Thread Index

There are 18509 messages in 6451 threads in the archives.

The mail message content can be searched from this page

- Date Index

- Re: [lammps-users] LAMMPS Compiling Problem, *Cun Zhang*, Feb 22 2011, 00:12
- [lammps-users] is the public svn version out of date?, *Jones, Reese*, Feb 21 2011, 22:23
- [lammps-users] silicon cantilever beam bending problem, *puroorava annapaneni*, Feb 21 2011, 16:01
- [lammps-users] Rerunning the simulation with Different Force Field, *Apoorv Kalyankar*, Feb 21 2011, 15:50
- [lammps-users] How to output per-molecule quantities?, Đ "Đ»ĐµĐ± ĐˆĐ²Đ°Đ½Đ¾Đ²Ñ‹Đ°Đ¸Đ¹ Feb 21 2011, 12:44
  - Re: [lammps-users] How to output per-molecule quantities?, *Axel Kohlmeyer*, Feb 21 2011, 12:49

Major Contributors:

- Steve Plimpton: staff member at Sandia Nat. Lab. http://www.sandia.gov/~sjplimp/
- Axel Kohlmeyer: Professor at Temple Univ. http://sites.google.com/site/akohlmey/
- You!

Mechanical Engineering

LAMMPS Overview: Potentials

- pair_style none - turn off pairwise interactions
- pair_style hybrid - multiple styles of pairwise interactions
- pair_style hybrid/overlay - multiple styles of superposed pairwise interactions

- pair_style airebo - AI-REBO potential
- pair_style born - Born-Mayer-Huggins potential
- pair_style born/coul/long - Born-Mayer-Huggins with long-range Coulomb
- pair_style buck - Buckingham potential
- pair_style buck/coul/cut - Buckingham with cutoff Coulomb
- pair_style buck/coul/long - Buckingham with long-range Coulomb
- pair_style colloid - integrated colloidal potential
- pair_style coul/cut - cutoff Coulombic potential
- pair_style coul/debye - cutoff Coulombic potential with Debye screening
- pair_style coul/long - long-range Coulombic potential
- pair_style dipole/cut - point dipoles with cutoff
- pair_style dpd - dissipative particle dynamics (DPD)
- pair_style dpd/tstat - DPD thermostatting
- pair_style dsmc - Direct Simulation Monte Carlo (DSMC)
- pair_style eam - embedded atom method (EAM)
- pair_style eam/opt - optimized version of EAM
- pair_style eam/alloy - alloy EAM
- pair_style eam/alloy/opt - optimized version of alloy EAM
- pair_style eam/fs - Finnis-Sinclair EAM
- pair_style eam/fs/opt - optimized version of Finnis-Sinclair EAM
- pair_style eim - embedded ion method (EIM)
- pair_style gauss - Gaussian potential
- pair_style gayberne - Gay-Berne ellipsoidal potential
- pair_style gayberne/gpu - GPU-enabled Gay-Berne ellipsoidal potential

- pair_style lubricate - hydrodynamic lubrication forces
- pair_style meam - modified embedded atom method (MEAM)
- pair_style morse - Morse potential
- pair_style morse/opt - optimized version of Morse potential
- pair_style peri/lps - peridynamic LPS potential
- pair_style peri/pmb - peridynamic PMB potential
- pair_style reax - ReaxFF potential
- pair_style resquared - Everaers RE-Squared ellipsoidal potential
- pair_style soft - Soft (cosine) potential
- pair_style sw - Stillinger-Weber 3-body potential
- pair_style table - tabulated pair potential
- pair_style tersoff - Tersoff 3-body potential
- pair_style tersoff/zbl - Tersoff/ZBL 3-body potential
- pair_style yukawa - Yukawa potential
- pair_style yukawa/colloid - screened Yukawa potential for finite-size particles

- pair_style gran/hertz/history - granular potential with Hertzian interactions
- pair_style gran/hooke - granular potential with history effects
- pair_style gran/hooke/history - granular potential without history effects
- pair_style hbond/dreiding/lj - DREIDING hydrogen bonding LJ potential
- pair_style hbond/dreiding/morse - DREIDING hydrogen bonding Morse potential
- pair_style lj/charmm/coul/charmm - CHARMM potential with cutoff Coulomb
- pair_style lj/charmm/coul/charmm/implicit - CHARMM for implicit solvent
- pair_style lj/charmm/coul/long - CHARMM with long-range Coulomb
- pair_style lj/charmm/coul/long/gpu - GPU-enabled version of CHARMM with long-range Coulomb
- pair_style lj/charmm/coul/long/opt - optimized version of CHARMM with long-range Coulomb
- pair_style lj/class2 - COMPASS (class 2) force field with no Coulomb
- pair_style lj/class2/coul/cut - COMPASS with cutoff Coulomb
- pair_style lj/class2/coul/long - COMPASS with long-range Coulomb
- pair_style lj/cut - cutoff Lennard-Jones potential with no Coulomb
- pair_style lj/cut/gpu - GPU-enabled version of cutoff LJ
- pair_style lj/cut/opt - optimized version of cutoff LJ
- pair_style lj/cut/coul/cut - LJ with cutoff Coulomb
- pair_style lj/cut/coul/cut/gpu - GPU-enabled version of LJ with cutoff Coulomb
- pair_style lj/cut/coul/debye - LJ with Debye screening added to Coulomb
- pair_style lj/cut/coul/long - LJ with long-range Coulomb
- pair_style lj/cut/coul/long/gpu - GPU-enabled version of LJ with long-range Coulomb
- pair_style lj/cut/coul/long/tip4p - LJ with long-range Coulomb for TIP4P water
- pair_style lj/expand - Lennard-Jones for variable size particles
- pair_style lj/gromacs - GROMACS-style Lennard-Jones potential
- pair_style lj/gromacs/coul/gromacs - GROMACS-style LJ and Coulombic potential
- pair_style lj/smooth - smoothed Lennard-Jones potential
- pair_style lj96/cut - Lennard-Jones 9/6 potential
- pair_style lj96/cut/gpu - GPU-enabled version of Lennard-Jones 9/6

-Most of these can be combined in a “hybrid” style
- Additionally, users can enter in potentials numerically or by writing a new module to LAMMPS

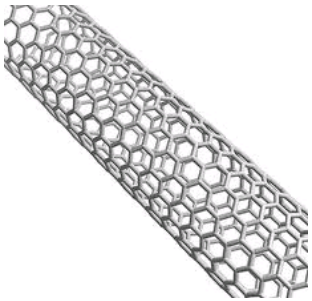
LAMMPS Overview: Potentials 2

FEATURES:

- Potentials for “soft” materials (biomolecules, polymers):

- Can simulate Colloids, bonded organic molecules, granular materials, etc.

- Potentials for “hard” materials (CNTs, Si, Metals, LJ, Charge):

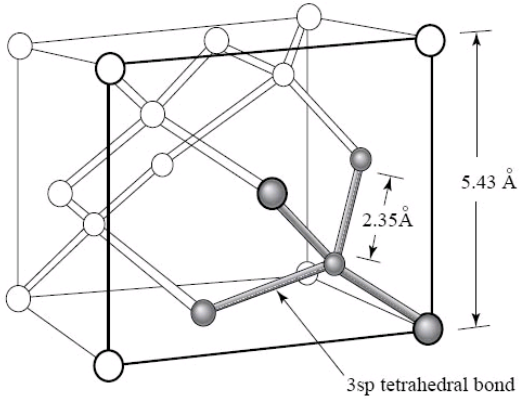


pair_style airebo - AI-REBO potential

Can simulate CNTs/hydrocarbons:

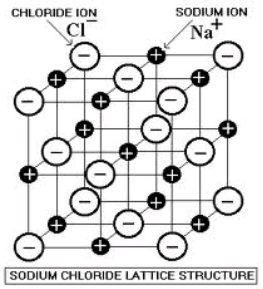
pair_style sw - Stillinger-Weber 3-body potential

Can simulate Si/Ge:



pair_style coul/long - long-range Coulombic potential

Can handle Coulomb, from Class:



$$\Phi = \frac{1}{2}\sum_{i}\sum_{i\neq j}\phi(r_{ij}) \qquad \Phi = \int_{R}^{\infty} 4\pi r^2 \phi(r) dr \rightarrow r^{-2} \rightarrow \int_{R}^{\infty} r^0 dr = \infty$$

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LAMMPS Installation

- LAMMPS can be downloaded from:

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

- Includes the current "build" (with both serial and parallel capabilities) and older builds.
- Also available are **Windows** serial and parallel versions:

- LAMMPS can be "installed" in **Windows** using Cygwin: http://www.cygwin.com/

Linux

- The current "build" has the most recent functionality. Consequently, it may be incompatible with old compilers/libraries.

Needed:

Serial

- **Desktop PC running (almost) any Linux OS.**
- **C++ compiler (GNU gcc or Intel icc)**: GNU installed by default in almost every Linux OS.

Parallel

- **Parallel computer (Cluster, GPU, etc.).**
- **MPI library (openmpi, impi, mpich) for parallel code**: Mpich and openmpi installed by default on most computing clusters.

LAMMPS Installation 2

- Detailed instructions here:

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

```
root@jason-desktop:/home/jason/lammps# ls
Johan            lammps-18Aug10.tar.gz  lammps.tar.gz  work
lammps-16Apr10   lammps-25Oct10         LJ
lammps-18Aug10   lammps2.tar.gz         log.lammps
```

root@jason-desktop:/home/jason/lammps# tar xvf lammps-18Aug10.tar.gz

- This unzips the LAMMPS program files to a folder called “lammps-18Aug10”

root@jason-desktop:/home/jason/lammps# cd ./lammps-18Aug10/src

- This moves to the “src” folder which has the source code files. Once here, there are a few options. To compile the code type:

root@jason-desktop:/home/jason/lammps/lammps-18Aug10/src# make machine

Where **machine** can be:

```
# mingw = Windows 32bit, cross-compiled on Linux, gcc-4.4.1, MinGW x-compiler
# mkl = Intel Cluster Tools, mpiicc, MKL MPI, MKL FFT
# odin = 1400 cluster, g++, MPICH, no FFTs
# openmpi = Fedora Core 6, mpic++, OpenMPI-1.1, FFTW2
# pgi = Portland Group compiler, pgCC, MPICH, FFTW
# power5 = IBM Power5+, mpCC_r, native MPI, FFTW
# qed = CSRI cluster, mpiCC, MPICH, no FFTs
# redsky - SUN X6275 with dual socket/quad core nodes, mpic++, openmpi, FFTW
# sdsc = SDSC BG/L machine, xlC, native MPI, FFTW
# seaborg = NERSC IBM machine, mpCC, native MPI, FFTW
# serial = RedHat Linux box, g++4, gfortran, no MPI, no FFTs
# serial_debug = RedHat Linux box, g++4, gfortran,  no MPI, no FFTs
# sgi = SGI Origin 350 64-bit, SGI MIPSpro CC, SGI MPI, SGI SCSL MP FFTs
# solaris = Sun box, c++, no MPI, no FFTs
# spirit = HP cluster 64-bit, mpicxx, native MPI, FFTW
# storm = Cray Red Storm XT3, Cray CC, native MPI, FFTW
# tacc = UT Lonestar TACC machine, mpiCC, MPI, FFTW
# tbird = Dell cluster with Xeons, Intel mpicxx, native MPI, FFTW
# tesla = 16-proc SGI Onyx3, g++, no MPI, SGI FFTs
# tunnison - 64-bit dual-core Linux cluster, mpic++, OpenMPI-1.1, FFTW2
# xt3 = PSC BigBen Cray XT3, CC, native MPI, FFTW
```

```
# altix = SGI Altix, Intel icc, MPI, FFTs from SGI SCSL library
# bgl = LLNL Blue Gene Light machine, xlC, native MPI, FFTW
# cygwin = Windows Cygwin, mpicxx, MPICH, FFTW
# encanto = NM cluster with dual quad-core Xeons, mpicxx, native MPI, FFTW
# fink = Mac OS-X w/ fink libraries, c++, no MPI, FFTW 2.1.5
# g++ = RedHat Linux box, g++4, gfortran, MPICH2, FFTW
# g++3 = RedHat Linux box, g++ (v3), Intel ifort, MPICH2, FFTW
# glory = Linux cluster with 4-way quad cores, Intel mpicxx, native MPI, FFTW
# jaguar = ORNL Jaguar Cray XT5, CC, native MPICH, FFTW
# lam = FreeBSD box, mpic++, Intel ifort, LAM/MPI, FFTW
# linux = RedHat Linux box, Intel icc, Intel ifort, MPICH2, FFTW
# mac = Apple PowerBook G4 laptop, c++, Intel ifort, no MPI, FFTW 2.1.5
# mac_mpi = Apple PowerBook G4 laptop, mpic++, gfortran, fink LAM/MPI, fink FFTW
 2.1.5
```

LAMMPS Installation 3

- The previous section will make LAMMPS with the standard “packages”. Additional packages can be included/excluded during installation, but may require additional libraries (fft, etc.).

asphere	aspherical particles and force fields
class2	class 2 force fields
colloid	colloidal particle force fields
dipole	point dipole particles and force fields
dsmc	Direct Simulation Monte Carlo (DMSC) pair style
gpu	GPU-enabled force field styles
granular	force fields and boundary conditions for granular systems
kspace	long-range Ewald and particle-mesh (PPPM) solvers
manybody	metal, 3-body, bond-order potentials
meam	modified embedded atom method (MEAM) potential
molecule	force fields for molecular systems
opt	optimized versions of a few pair potentials
peri	Peridynamics model and potential
poems	coupled rigid body motion
reax	ReaxFF potential
replica	multi-replica methods
shock	methods for MD simulations of shock loading
srd	stochastic rotation dynamics (SRD)
xtc	dump atom snapshots in XTC format

- This customizability ensures that LAMMPS (in one form or another) **can be run on virtually any computer**.
- Result should be an executable located in the src/lmp_machine, where machine depends on how you compiled (for me it’s lmp_openmpi).

LAMMPS Example: How to Run

Steps:

1) Set your path to the location of the LAMMPS executable:

export PATH = /home/jason/lammps/lammps-16Apr10/src

In this "./src/" directory is the LAMMPS executable. For me: **"/src/lmp_serial"**

2) Put the example files into a directory, say:

/home/jason/lammps/LJ/0press_alat

```
root@jason-desktop:/home/jason/lammps/LJ/crystal/0press_alat# ls
in.LJAr.alat   LJ.4x4x4.in.data   tau_T10_tau_P10   tau_T1_tau_P10
```

Input Script Input Structure

3) Run the executable with:

```
root@jason-desktop:/home/jason/lammps/LJ/crystal/0press_alat# nohup lmp_serial < in.LJAr.alat &
```

This command runs LAMMPS in background and gives you back control of the command terminal. Type "top" to check if LAMMPS is running:

```
  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
31096 root      25   0  6328 1980 1416 R 99.8  0.2  29:27.65 lmp_serial
    1 root      16   0  1568  524  456 S  0.0  0.1   0:04.87 init
    2 root      34  19     0    0    0 S  0.0  0.0   0:00.00 ksoftirqd/0
    3 root      RT   0     0    0    0 S  0.0  0.0   0:00.00 watchdog/0
    4 root      10  -5     0    0    0 S  0.0  0.0   0:00.75 events/0
```

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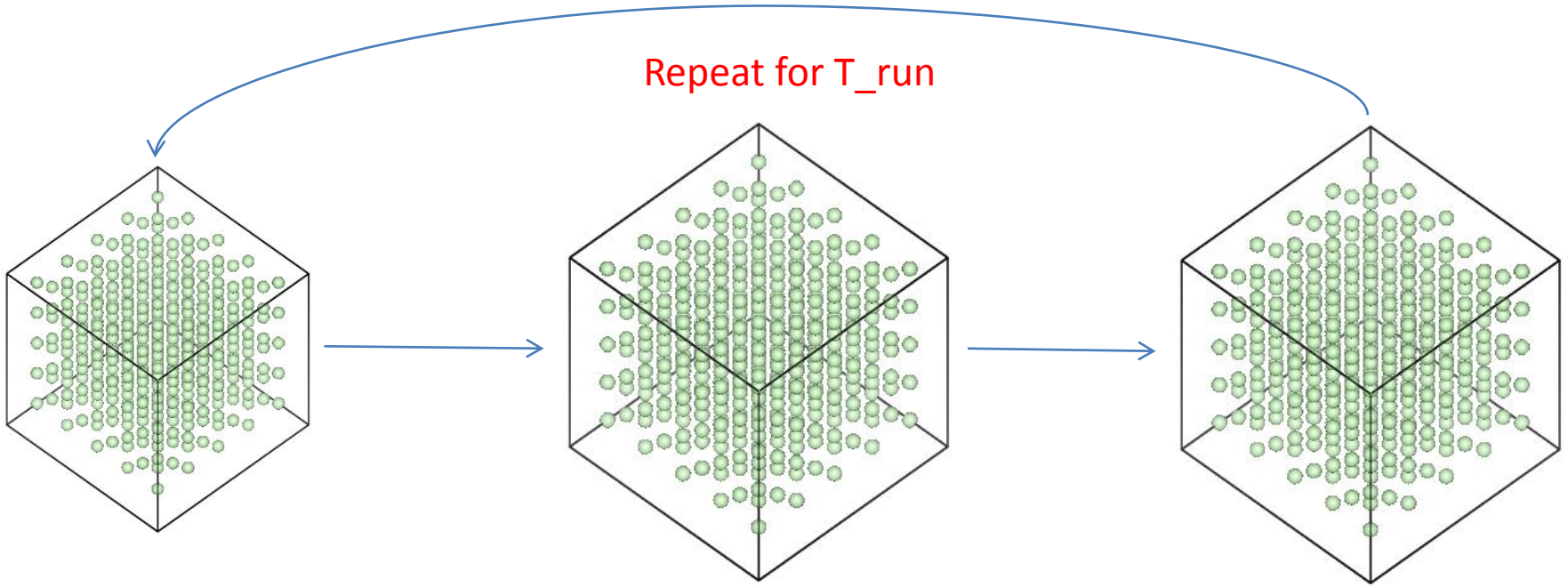
LAMMPS Example Code

Input file (has MD information): in.LJAr.alat Input Structure: LJ.4x4x4.in.data

What happens:

1) Measures 0 pressure lattice constant (alat) for 4x4x4 supercell of FCC Ar (256 atoms) using NPT ensemble.
2) Measure constant volume specific heat using formula: $\langle T \rangle = \left[\frac{\langle (E - \langle E \rangle)^2 \rangle}{3(N-1)k_B c_v} \right]^{1/2}$
3) Do 1) and 2) for T_run = 10...80K



NPT heat to allow cell expansion to 0 Press at T_run.

NPT data collection to measure <alat>

NVT to measure cv

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LAMMPS Example I

```
#-------------------------------------------------------------------------------------------------
###################################MEASURE 0 PRESS ALAT#############################################
#-------------------------------------------------------------------------------------------------
clear
#------------READ STRUCTURE---------------------------------------------------------------------
units           lj                  ##Use LJ units sigma_Ar, eps_Ar, tau_Ar
atom_style      atomic                  ##Specifies how many columns in data in
read_data       LJ.4x4x4.in.data            ##Specifies input data file with "atomic"
#read_restart   ljNVE.restart.1000000
mass            1  1.0                  ##Specifies mass again, not really needed
group           Ar type = 1             ##Gives a label to atome type=1 "Ar"
#------------LJ POTENTIALS----------------------------------------------------------------------
pair_style      lj/cut 2.5              ##LJ with cutoff a=2.5
pair_coeff      1 1 1.0 1.0             ##atomi atomj epsilon sigma
pair_modify          shift yes              ##Shift PE at cutoff to 0.0

##USED TO SPECIFY MULTIPLE SPECIES
##pair_style        lj/cut 2.5
##pair_coeff        1 2 1.0 1.0
##pair_modify        shift yes

##pair_style        lj/cut 2.5
##pair_coeff        2 2 1.0 1.0
##pair_modify        shift yes

#pair_modify    tail no             ##This is default so not needed
#------------LJ PARAMETERS----------------------------------------------------------------------
variable        kB      equal 1.3806504e-23         # [J/K] Boltzmann
variable    sigma_Ar    equal 3.4e-10       # m
variable    eps_Ar      equal 1.67e-21      # J
variable    mass_Ar equal 6.63e-26      # kg
variable    tau_Ar      equal 2.1423e-12        # s
#------------THERMO PARAMETERS------------------------------------------------------------------
variable        T_melt  equal 300*(${kB}/${eps_Ar})
variable    T_OK        equal 0.001
#variable   T_run       equal 15*(${kB}/${eps_Ar})
#variable       V       equal vol
variable    dt      equal 0.002
variable    run_length  equal 500000
variable    Tau_T       equal 1.0
variable    Tau_P       equal 10.0
variable    seed        equal 99999
#------------SAMPLE PARAMETERS------------------------------------------------------------------
variable        p       equal 100           # correlation length
variable        s       equal 10            # sample interval
variable        d       equal $p*$s             # dump interval
```

in.LJAr.alat

What happens:

1) Input structure
2) Interaction potential
3) Simulation variables

Continued…

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LAMMPS Example 2

```
#START LOOP 1

    label loop1
    variable a loop 8
    variable T_run index 0.082670659 0.165341317 0.248011976 0.330682635 0.413353293 0.496023952 &
    0.578694611 0.661365269

    log     log_$a.lammps

    #------------START NPT HEAT ------------------------------------------------------------------

        reset_timestep      0

            ##IF FIRST T_run CREATE INITIAL VEL

                ##if "${a}<2" then "velocity all create ${T_run} ${seed} rot yes dist gaussian"
                velocity all create ${T_run} ${seed} rot yes dist gaussian

    ##START
            ##RUN A PREPARATION NPT
                ##SET ENSEMBLE TO NPT

                fix             1 all npt temp ${T_run} ${T_run} ${Tau_T} iso press 0.0 ${Tau_P}
                thermo_style    custom step temp press vol etotal pe ke
                thermo      1000

                ##OPTIONAL DUMP POSITIONS

                ##dump          xyz all xyz ${run_length} npt_heat_$a.dump

                run                 50000
              #run      1000
                unfix           1
    ##STOP
```

What happens:

1) Run an NPT to initialize

Continued…

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LAMMPS Example 3

```
#----------CALCULATE AVG CELL SIZE----------------------------------------------------------

##START
        ##RUN NPT FOR CELL SIZE
            fix             1 all npt temp ${T_run} ${T_run} ${Tau_T} iso press 0.0 ${Tau_P}

            ##SET myLx EQUAL TO THE X_DIM BOX SIZE

            variable        myLx equal xhi-xlo

            ##CREATE A FIX WHICH AVERAGES THE X-DIM BOX SIZE OVER TIME

            fix             myLx all ave/time ${p} ${s} ${d} v_myLx file Lx.profile$a

            ##SET ANOTHER VARIABLE myLx2 EQUAL TO THE TIME AVERAGED X-BOX DIM

            variable        myLx2 equal f_myLx

            ##DO FOR Y AND Z DIRECTIONS AS WELL

            variable        myLy equal yhi-ylo
            fix             myLy all ave/time ${p} ${s} ${d} v_myLy file Ly.profile$a
            variable        myLy2 equal f_myLy
            variable        myLz equal zhi-zlo
            fix             myLz all ave/time ${p} ${s} ${d} v_myLz file Lz.profile$a
            variable        myLz2 equal f_myLz

        ##REPORT THERMO DATA EVERY thermo NUMBER TIME STEPS

            thermo_style    custom step temp press vol etotal pe ke #v_myLx2 v_myLy2 v_myLz2
            thermo      1000

        ##RUN THE ENSEMBLE FOR THIS MANY TIME STEPS

            run         100000
          #run          5000

        ##UNLOCK THE DUMP AND FIX COMMANDS SO THEY CAN BE USED AGAIN LATER

            unfix           1
##STOP
```

What happens:

1) Run in NPT
2) Time average Lx, Ly, Lz

Continued…

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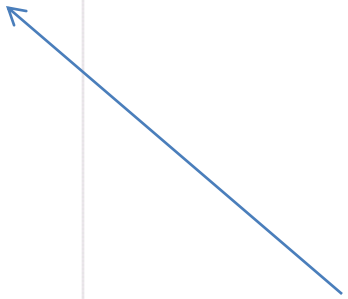
LAMMPS Example 4

```
##START
        ##THE FINAL TEIM AVG myL(x,y,z)2 USED TO RELAX SIM BOX TO ABOVE AVG LATTICE CONTANTS

            fix             deform all deform 1 x final 0.0 $(myLx2) y final 0.0 $(myLy2) z final 0.0 $(myLz2) units box

        ##RELAX THE SIM BOX OVER THIS MANY TIME STEPS

            run         10000
            #run            1000

        ##UNLOCK FIXED AND COMPUTES TO USE LATER

            unfix       deform
            unfix       myLx
            unfix               myLy
            unfix               myLz
##STOP

#------------STOP NPT HEAT ------------------------------------------------------------------
```



What happens:

1) Sim. Box dimensions are changed to <Lx>, <Ly>, <Lz>

Continued…

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LAMMPS Example 5

```
#------------ START NVT equil ----------------------------------------------------------

##START
        ##RUN A PREPARATION NVT
            ##SET ENSEMBLE TO NVT
            fix             1 all nvt temp ${T_run} ${T_run} ${Tau_T}
            thermo_style    custom step temp press vol etotal pe ke
            thermo      1000
            run                 50000
          #run          1000
            unfix       1
##STOP

##START
        ##COLLET NVT DATA FOR Cv
            fix             1 all nvt temp ${T_run} ${T_run} ${Tau_T}
            thermo_style    custom step temp press vol etotal pe ke
            thermo      1000
            run                 100000
          #run               5000
            unfix               1
##STOP

next T_run
next a
jump in.LJAr.alat loop1

#END LOOP 1
```

What happens:

1) Short NVT run to initialize.
2) Data collection NVT run to measure Cv
3) Loop ends for given T_run, starts over.

END

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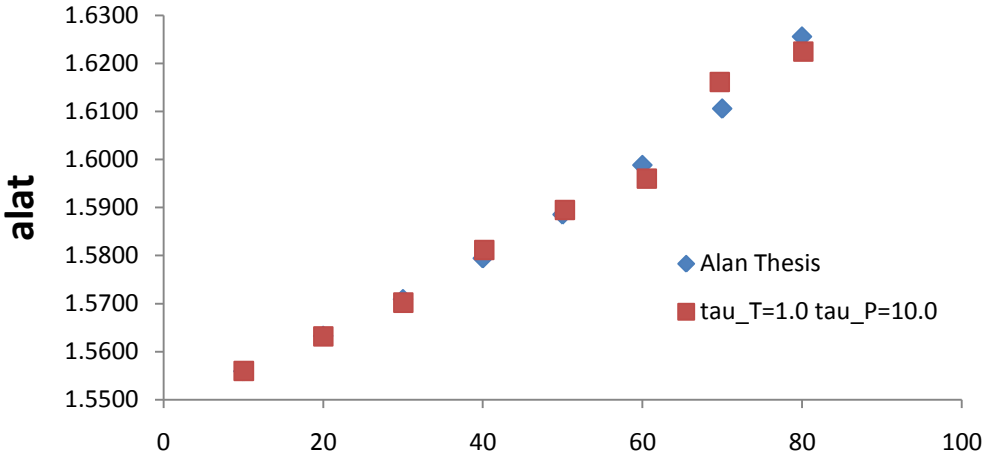
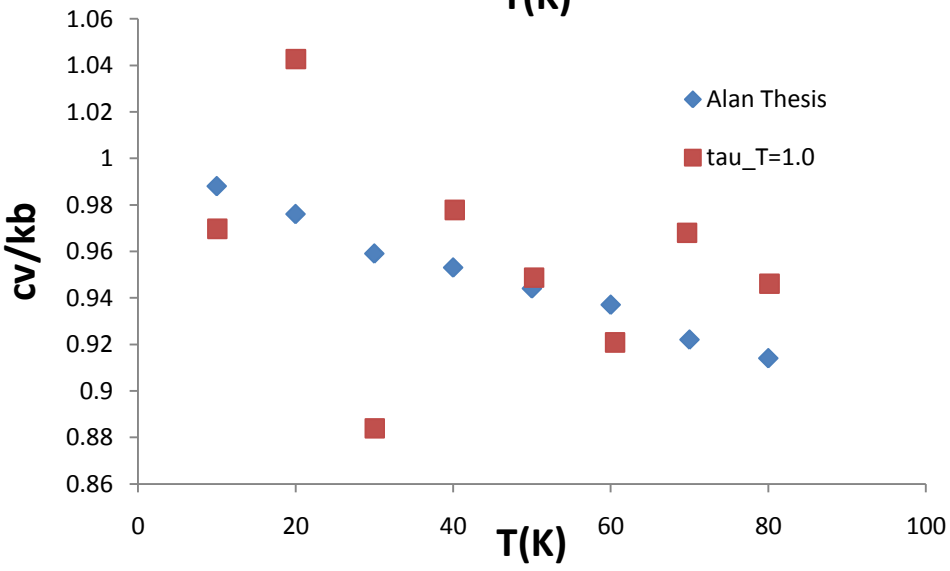
LAMMPS Example Results

Explanation for differences:

1) Thermo sampling rate (more data to average cv).
2) Average over different initial conditions (how could you do this?).
3) Vary tau_T to see if this has an effect.
4) Increase the equilibration times between NVT and NPT data collection segments.

You can easily automate all of these (and much more).





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LAMMPS Performance

- Using the Lecture Example code, I get the following performance:

LAMMPS:

Ubuntu 9.0, 2.0 GHz CPU, 1 GB RAM, 256 atoms, NPT, neighbor listing:

Rate = 1000 steps/s

Larger systems will scale N*rate because of neighbor listing. Can be even faster using parallel capabilities.

My LJ Code:

Ubuntu 9.0, 2.0 GHz CPU, 1 GB RAM, 256 atoms, NPT, NO neighbor listing:

Rate = 70 steps/s

Larger systems will scale as ~N^2 since no neighbor listing.

LAMMPS Modifications

- This section describes how to add/modify the LAMMPS source code:

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

- LAMMPS is designed on a modular fashion using C++.
  http://www.cplusplus.com/doc/tutorial/

- Hi-level structure uses classes, functions are class methods and use simple array, vectors, numbers. http://www.cplusplus.com/reference/stl/vector/vector/
- Creating a new class requires new.cpp and new.h. Best way to understand is to look at existing classes (like compute_temp.cpp and compute_temp.h).
  http://www.cplusplus.com/doc/tutorial/classes/

- If worthy, new features are encouraged to be submitted to LAMMPS developers.

LAMMPS Matlab Post-Processing

- There are many ways to post-process the LAMMPS output:

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

- Ability to read *.dump files one at a time, or an entire run full.
- Read RDF files
- Read *.log files to easily plot thermo data