

Homework #2 – Running a simulation with MSE627-MD

**Objective:** Become familiar with the MSE627-MD code, pick an appropriate timestep for integration, understand the partitioning of the thermal energy between the potential and kinetic energies, and think about the melting process under conditions of constant volume.

1. Compile the code using the makefile. You do not need to edit makefile if you compile the code at blue.unix.virginia.edu. To execute the makefile type *make*. One advantage of using a makefile is that if you edit one routine you do not have to recompile everything.\* You should end up with an executable *mse627*. The executable will appear in the same directory where the source code is.
2. Create directory for the simulation, copy all input files (from *hw2-input* directory) and the executable to this directory. I made an FCC crystal of  $5 \times 5 \times 5$  unit cells (*Ar.data*) for you. It is composed of 500 atoms. Parameters for Lennard-Jones potential are chosen to be appropriate for Ar ( $\epsilon = 0.0103$  eV and  $\sigma = 3.405$  Å as defined in *Eftab\_pair.f*). You should be able to run the program without making any changes to the input files. Before running the code, you should create a subdirectory *data* in the directory where you are running the code (see the last line of *md.rc*).
3. Run the code. Examine the code and the output files to see if everything makes sense. If you have questions, ask me, preferably by sending your questions to the class mailing list so that everyone can see the questions, try to answer them, and see the answers. I tested the code and found that it takes ~6 minutes to run 5000 steps for 500 Lennard-Jones atoms on blue.unix.
4. Make plots of the potential energy and the force for a pair of atoms on the same graph (you will need to uncomment “open”, “write”, and “close” statements in *Eftab\_pair.f* if they are commented out). Once you have plotted the potential and the force for a pair of atoms, answer the following questions (use handouts with an equation for the Lennard-Jones potential).
  - A. What is the value of the equilibrium distance  $r_e$  between two atoms? Express the equilibrium distance through the parameters of the potential,  $\epsilon$  and  $\sigma$ .
  - B. What is the value of the FCC lattice constant that corresponds to the equilibrium interatomic distance?
  - C. Evaluate the force constant,  $k$ , within the linear (harmonic) approximation near  $r_e$ . That is, assume  $V(r) = \frac{1}{2} k (r-r_e)^2$  for small  $r-r_e$  and calculate  $k$  that would provide the closest approximation for the Lennard-Jones potential (*this is an optional questions for undergraduate students*).

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\* If you change common.h or parameters.h you do have to recompile all the files since these files are “inserted” to most of the subroutines. In this case you have to delete all object files (rm \*.o) and then recompile the code.

5. Perform a simulation with periodic boundary conditions (LIDX=LIDY=LIDZ=1 in *md.input*) at a given temperature. Define the temperature in *md.input* (QTEM) and introduce the initial temperature through the velocity distribution (KFLAG=2 in *md.input*).

To add variability, each student is assigned a different temperature:

Duvall, Kevin	20 K
Klein, Christoph	50 K
Wu, Xiang	80 K
Shih, Cheng-Yu	120 K
Conti, Rebecca	150 K
Zemer, Hagit	180 K
Baker, Christopher	10 K
Bhattacharyya, Jishnu	30 K
Duska, Christopher	40 K
Feng, Xuhui	60 K
Lawlor, Thomas	70 K
Le, Nam	90 K
McClimon, John	100 K
O'Donnell, Sarah	110 K
Ramalingam, Gopalakrishnan	130 K
Richards, Bradley	140 K
Ryan, Herbert	160 K
Schaible, Micah	170 K
Schindelholz, Eric	190 K
Smoyer, Justin	200 K
Srinivasan, Jayendran	300 K
Wittmaack, Bernard	400 K
Srinivasan, Jayaprakash	220 K
Lupton, Max	240 K
Long, Karen	10 K
Owens, Tyler	85 K

Choose an appropriate time-step for the Nordsieck integrator for the simulation. As you noticed in your homework #1, choosing a good time-step in MD is an empirical task. Try one value and examine the energy conservation. Double and halve the value and reexamine the energy conservation. Iterate until you are happy with your choice. Test runs can be ~10 ps long.

6. Once you have picked your 'best' time-step, identify it in your report and run a longer simulation for 50 ps using your best time-step. Plot the kinetic, potential and total energies, as well as temperature.

*Discuss the observed values and time dependences of the energies* - why the average potential (kinetic, total) energy is equal to XX eV? Are the average potential and kinetic energies equal to each other and why? When discussing the values of energies and temperature relate them to the equipartition principle and virial theorem briefly discussed in class.

7. Plot the initial and final (at time 50 ps) configurations for the simulation with your best time-step). You can use your favorite plotting program to plot data points for xy (or xz or yz) coordinates but not the connecting lines. Or use “scatter plot” option if your graphic program has one. You can also consider one of the available free visualization packages, e.g. RasMol: <http://www.umass.edu/microbio/rasmol/>  
<http://www.bernstein-plus-sons.com/software/rasmol/>

You can use files that are written to subdirectory *data* by *Swrite.f*. In the current version coordinates are in 3<sup>rd</sup>, 4<sup>th</sup>, and 5<sup>th</sup> columns of the files. You can change format of the output files to suit your graphic program by editing *Swrite.f*. Discuss the differences between the initial and final configurations. ***Did melting occur?***

8. Find the melting temperature for Ar in literature and relate to your observations (*optional for undergraduate students*).

Do not hesitate to send your questions to the mailing list.

**Do not leave this homework for the last evening before the due date!**

We will summarize your results in class.

**Happy Computing!**