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 rivanna cluster. 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 5×5×5 unit cells (Ar.data) for you. It is composed of 500 atoms. Parameters for Lennard-Jones potential are chosen to be appropriate for Ar ($\varepsilon = 0.0103$ 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 e-mail list so that everyone can see the questions and answers. Please try to answer or discuss questions posted by other students.

4. Make plots of the potential energy and 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, $\varepsilon$ 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).

* 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 \textit{md.input}) at a given temperature. Define the temperature in \textit{md.input} (QTEM) and introduce the initial temperature through the velocity distribution (KFLAG=2 in \textit{md.input}).

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

- Matthew Barone 20 K
- Jeffrey Braun 50 K
- Ben Canty 80 K
- Yuan Gao 120 K
- Jennifer Hays 150 K
- Qishen Huang 180 K
- La Shawn Johnson 200 K
- Robert Klein 30 K
- Chao Liu 40 K
- Qingchang Liu 60 K
- Rouzbeh Rastgarkafshgarkolaei 70 K
- Chester Szwejkowski 90 K
- Alexander Yang 100 K
- Yue Zhang 110 K
- Zhongmin Zhang 130 K

Choose an appropriate time-step for the Nordsieck integrator for the simulation. As you noticed in your homework #1 & 2, 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 ~10-20 ps long.

6. Once you have picked your 'best' time-step, identify it in your report and run a longer simulation for 100 ps using your best time-step. Plot the kinetic, potential and total energies, as well as temperature.

\textbf{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? Why are they equal (or not equal) to each other?
7. Plot the initial and final (at time 100 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.,

AtomEye:
http://li.mit.edu/Archive/Graphics/A/

Open Visualization Tool by Alexander Stukowski
http://www.ovito.org/

RasMol:
http://www.umass.edu/microbio/rasmol/
http://www.bernstein-plus-sons.com/software/rasmol/

or any other software you can find.

You can use files that are written to subdirectory data by Swrite.f. In the current version
coordinates are in 3rd, 4th, and 5th 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 it to your computational results
(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!