MSE 301 Integrated Computational Materials Engineering
Homework 2: Molecular Dynamics
Due in class on Tuesday March 12

A. **<u>Conceptual Short Answer Questions:</u> (35 points, 5 points each)**

1. A typical potential curve for most materials looks like the one shown in Figure 1. Referring to the curve, why do most materials expand with increasing temperature?

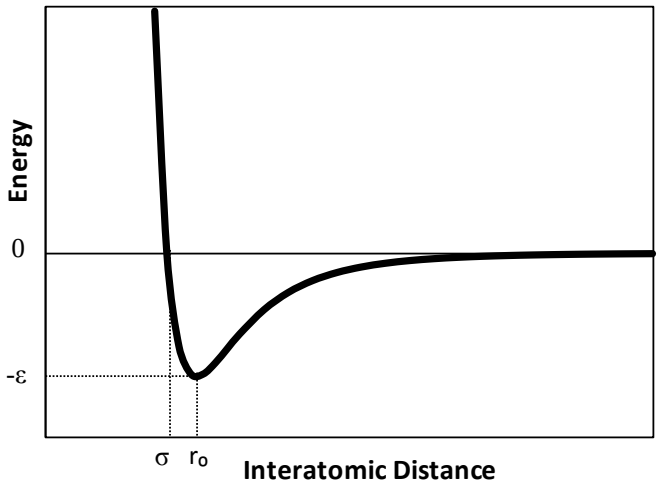

Figure 1. Schematic of the Lennard-Jones Pair Potential

2. Compare the three primary potential classes (Embedded Atom Method, Tersoff, and Ionic Solids). Provide the materials classes for each as well as how (mathematically) the potential accounts for the important features of that material class.

3. Explain the two types of errors which occur in computer simulations such as MD. Which one dominates at long time steps and why?

4. If we increase the velocities of the atoms in a system by two times, by how many times will the corresponding system temperature increase?

5. Draw the general features of a MSD function with simulation time when a crystalline solid is melted and becomes a liquid. Explain this behavior.

6. Predict the first peak in the diagram of the radial distribution function for a simple cubic solid and an FCC solid.

7. Describe at least 3 features of periodic boundary conditions. Also give two examples of situations where you should use periodic boundary conditions and one where you should not.

B. **Calculations: (65 points total)**

Responses to Part B questions should be typed in report format. Include any generated plots which are requested as well as discussion/interpretation of your results.

1. MD Simulation of a Lennard-Jones Liquid (30 points)
    i. Simulate liquid Argon (80 K)
    ii. Begin with a 32 atom periodic cell input (from the second in-class lab)
    iii. Quantities to compute:
        1. pressure, temperature, energy per particle, diffusion coefficient
        2. Did the temperature change during the simulation?
    iv. Extend the system to 128 atoms, but maintain the same particle density
        1. Compare the results of the two simulations
    v. Decrease the temperature to 40K (use whichever cell from above is appropriate). What changes in the system are observed compared with the higher temperature system?
2. Melting of Aluminum (35 points)
    i. Simulate the melting of both bulk solid Aluminum and a 4000 atom Al cluster
    ii. Determine the equilibrium total energy of the systems at temperatures from 0K to 1600K in 100K intervals
    iii. Generate caloric curves to indicate the melting temperature of the systems
    iv. How do the temperatures compare with each other and with the experimental melting temperature? Explain why the differences are observed.