24-623/12-623 2017 HW#1

Total points: 50
Assigned: August 30, 2017.
Due: September 14, 2017, midnight to Canvas. Please use the Canvas to ask questions of the instructor or the other students.

1. (20 points) Download the program start.cpp and the file 5input.txt from Canvas. This program shows examples of input/output and data structures. If you are not familiar with programming, spend some time figuring out what this program does and how it works.

Modify start.cpp so that it:

(i) Evaluates the polynomial $2x^6 - 3x^4 + 5x^2 - 7$ using both "int" and "double" variables. In your submission, describe the most computationally efficient way to evaluate this function.

(ii) Determines if the integer is prime. In your submission, explain how your algorithm works.

Run the program for the following set of integers: (-28, 0, 11, 45, 397, 677, 951, 2552, 6449, 7411, 7412). Compare and explain what happens when you evaluate the polynomial using "int" or "double" variables. Submit your output and a discussion of any issues related to the results that might be of interest.

2. (9 points) Find two papers in the scientific literature of interest to you that use either molecular dynamics or Monte Carlo simulations. Include these papers in your submission. Write one typed page explaining why you chose these papers.

3. (6 points total)

(a) (3 points) Calculate how many water molecules are in spherical droplets with diameters of 1 nm, 10 nm, and 100 nm.

(b) (3 points) Assume that you will treat each water molecule as three point masses that are rigidly connected (i.e., the oxygen atom and two hydrogen atoms in a given water molecule do not interact). How many distinct pair interactions are there in each of the droplets from (a)?

4. (15 points total) The Lennard-Jones (LJ) potential is given by

$$u(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right], \tag{1}$$

where ϵ and σ are the energy scale and the length scale. The LJ mass scale is m, the mass of one atom. Equation (1) describes how two isolated atoms interact. It does not describe the environment experienced by an atom in a crystal. The energy of an atom i in a crystal can be found by summing over the contributions of all other atoms:

$$U_i = \frac{1}{2} \sum_{j \neq i} u(r_{ij}). \tag{2}$$

The stable crystal structure of LJ solids is face-centered cubic (fcc). In this case, Eq. (2) can be written as a function of the nearest neighbor distance, r_{nn}, as

$$U_i(r_{nn}) = 2\epsilon \left[A_{12} \left(\frac{\sigma}{r_{nn}} \right)^{12} - A_6 \left(\frac{\sigma}{r_{nn}} \right)^{6} \right], \tag{3}$$

where $A_{12} = 12.13$ and $A_6 = 14.45$.

(a) (5 points) Show Eqs. (1) and (3) together on a plot of (u or U_i)/ϵ vs. (r or r_{nn})/σ. Based on the shapes of the two curves, describe how the environment experienced by an atom in each will be different.

(b) (4 points) Analytically determine the value of r (or r_{nn}) at which the energy is zero and at which the energy is a minimum for each of Eqs. (1) and (3) in terms of the LJ scales. Show these points on the plot from part (a).

(c) (2 points) Determine the LJ heat capacity scale [i.e., the combination of the mass, energy, and length scales, and the Boltzmann constant (k_B) that gives units of J/kg-K].

(d) (4 points) A molecular dynamics simulation for LJ argon run at a temperature of 20 K predicts a heat capacity of 450 J/kg-K. Determine the dimensionless temperature and dimensionless heat capacity corresponding to this simulation. What are the corresponding temperature and heat capacity for LJ krypton based on these dimensionless values?

For argon: $\epsilon = 1.67 \times 10^{-21}$ J, $\sigma = 3.40 \times 10^{-10}$ m, and $m = 6.63 \times 10^{-26}$ kg.
For krypton: $\epsilon = 2.24 \times 10^{-21}$ J, $\sigma = 3.65 \times 10^{-10}$ m, and $m = 13.9 \times 10^{-26}$ kg.
$k_B = 1.3806 \times 10^{-23}$ J/K.