24-623 2010 HW#1

Assigned: January 11, 2010.
Due: January 20, 2010 at the beginning of class. Please use the Blackboard discussion board to ask questions of the instructor or the other students.

1. (10 points) Download the program start.cpp and the file input.txt from Blackboard. This program shows some 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:

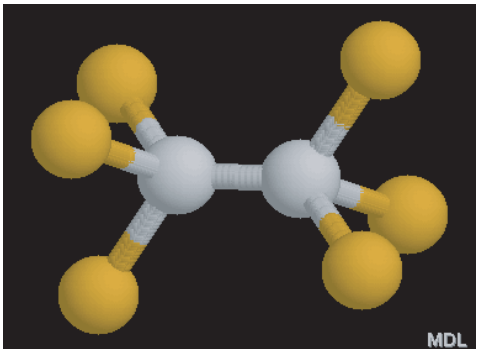
(i) The program evaluates the polynomial $2x^6 - 3x^4 + 4x^2 - 3$. In your submission, describe the most computationally efficient way to evaluate this function.

(ii) The program checks to see if the integer is prime. In your submission, explain how your algorithm works.

Run the program for the following set of integers: (11, 28, 45, 397, 677, 951, 2552, 6447, 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. (5 points) Water at ambient conditions has density 1000 kg/m^3. At supercritical conditions ($T = 400$°C and $p = 230$ bar), the density is reduced to 100 kg/m^3. Your computational resources allow you to perform simulations containing 10,000 water molecules. Assuming that your simulation domain is a cube with side length L, find L for simulations at ambient and supercritical conditions. How much would L change if you could perform simulations with 10 times as many molecules?

3. (5 points) Write down the form of a potential suitable for modeling an Si_2F_6 molecule, as rendered below. Determine how many terms would appear in each of the summations.



4. (10 points) The Lennard-Jones (LJ) potential is given by

$$\phi(r) = 4\epsilon_{\mathrm{LJ}} \left[\left(\frac{\sigma_{\mathrm{LJ}}}{r} \right)^{12} - \left(\frac{\sigma_{\mathrm{LJ}}}{r} \right)^{6} \right], \tag{1}$$

where ϵ_{LJ} and σ_{LJ} are the energy scale and the length scale. (The LJ mass scale is m_{LJ}, 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:

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

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

$$\Phi_i(r_{nn}) = 2\epsilon_{\mathrm{LJ}} \left[A_{12} \left(\frac{\sigma_{\mathrm{LJ}}}{r_{nn}} \right)^{12} - A_6 \left(\frac{\sigma_{\mathrm{LJ}}}{r_{nn}} \right)^{6} \right], \tag{3}$$

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

(a) (3 points) Show Eqs. (1) and (3) together on a plot of (ϕ or Φ_i)/ϵ_{LJ} vs. (r or r_{nn})/σ_{LJ}. 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) (3 points) Determine the LJ thermal conductivity scale [i.e., the combination of the mass, energy, and length scales, and the Boltzmann constant (k_{B}) that gives units of W/m-K].

$\epsilon_{\mathrm{LJ}} = 1.67 \times 10^{-21}$ J, $\sigma_{\mathrm{LJ}} = 3.40 \times 10^{-10}$ m, $m_{\mathrm{LJ}} = 6.63 \times 10^{-26}$ kg, and $k_{\mathrm{B}} = 1.3806 \times 10^{-23}$ J/K.