24-623/12-623 2015 HW#3

Total points: 50
Assigned: September 30, 2015.
Due: October 15, 2015, 8 PM to Blackboard. Please use the Blackboard discussion board to ask questions of the instructor or the other students.

1. (10 points) In HW#1, you calculated (i) how many water molecules are in droplets with diameters of 1 nm, 10 nm, and 100 nm, and (ii) the number of distinct pair interactions in each of the droplets assuming that each water molecule could be modeled as three rigidly-connected point masses.

Now, estimate the number of distinct pair interactions in each droplet for cutoff radii of (a) 1 nm, (b) 2 nm, and (c) 5 nm. Base your calculation on the center of mass of the molecules (i.e., if the center of masses of two molecules fall within the cutoff radius, then all the point masses on each molecule interact). Make sure that you have the correct number of molecules to start.

2. (25 points) In this exercise, you will extend the functionality of your MD code. The end task is to model an LJ fluid in the NVE ensemble. Initial dimensionless coordinates for a 256-atom liquid system in a cubic simulation cell of side length 6.8 are available in the file liquid256.txt on Blackboard. Modify your MD code so that it:

- Randomly initializes the particle velocities in a manner that gives the system zero total momentum.
- Incorporates the continuous force, continuous energy cutoff scheme with a dimensionless cutoff of 2.5.
- Calculates the instantaneous temperature and pressure.
- Applies periodic boundary conditions and the nearest image convention so that you can model bulk systems (you will need to define the system size as a variable in your code).

You will implement the NVT ensemble in HW#4. Don't do it now.

Submit your code electronically and provide plots and written explanations showing the following for the 256-atom liquid LJ phase at a steady-state argon temperature of 100 K:

- Time variation of kinetic energy, potential energy, total energy, temperature, and pressure for 200 units of LJ time (i.e., 100,000 time steps). **The total energy should be conserved.**
- Conservation of momentum in the x, y, and z directions.

3. (15 points) Perform NVE simulations to determine the zero-pressure liquid density (in kg/m^3) at an argon temperature of 100 K. Explain what you did using words, plots, tables, etc. Just giving the answer is not sufficient.

BONUS (10 points)

Repeat Problem 3 for the continuous energy (but not continuous force) cutoff scheme. Explain why the density is different.