24-623 2010 HW#3

Assigned: February 3, 2010.
Due: February 17, 2010 at the beginning of class. Please use the Blackboard discussion board to ask questions of the instructor or the other students.

1. (20 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. A starting file for a 256-atom liquid system is available on Blackboard. The simulation cell size for that system is 6.8. Modify your code so that it:

- initializes the particle momenta (randomly or according to some distribution function - indicate what you did)
- incorporates the continuous force, continuous energy cutoff scheme
- 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#5. Don't do it now.

Provide plots and written explanations showing the following for the 256-atom liquid LJ phase at an 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

Do not submit your code.

2. (10 points) Perform NVE simulations to determine the following (5 points each):

- the zero-pressure liquid density (in kg/m^3) at an argon temperature of 100 K
- the argon density (in kg/m^3) at which the system displays near-ideal gas behavior

Explain what you did using words, plots, tables, etc. Just giving the answer is not sufficient.

BONUS WORK:

(5 points) Compare the pressure predicted by the two equations given in class.