24-623 2010 HW#5

Assigned: March 4, 2010.
Due: April 2, 2010 by 5 PM to McGaughey's mailbox. Please use the Blackboard discussion board to ask questions of the instructor or the other students.

In this homework, you will extend the functionality of your LJ MD code so that it can operate in the NVT ensemble. Perform your simulations using the 256-atom liquid LJ system provided in HW#3. You will then modify the code to perform NVT MC simulations. For all problems on this homework, make sure that your system has equilibrated before extracting data.

1. (20 points) Modify your MD code so that it controls temperature using the Nose-Hoover scheme discussed in class and summarized in the file NVT.pdf on Blackboard.

(a) Plot the average pressure as a function of density, ρ, for 950 kg/m^3 $< \rho <$ 1150 kg/m^3 at an argon temperature of 100 K. Estimate the density that gives zero pressure. Explain how you determined when your system is equilibrated.

(b) The thermodynamic temperature in the NVT ensemble is given by

$$\langle T \rangle = \left[\frac{\langle (E - \langle E \rangle)^2 \rangle}{3(N-1)k_{\mathrm{B}}c_v} \right]^{1/2}.$$

Run a sufficiently long simulation so that $\bar{T} = \langle T \rangle = 100$ K, then use the energy fluctuations to find the specific heat. Report the result in J/kg-K for argon. Note that $3c_v$ is the specific heat per atom. Explain what you did using words, plots, tables, etc. Just giving the answer is not sufficient.

2. (20 points) Modify your MD code so that it can also perform Metropolis MC NVT simulations. Ideally, your code will have the ability to perform either MD or MC, depending on one parameter that you specify at the beginning of the run. Repeat (a) and (b) from the first problem, and compare your answers. Explain how you determine when your MC simulation is equilibrated. From the standpoint of computational efficiency, do you recommend using MD or MC to predict specific heat? Why?

Note the in MC simulation, you don't calculate the total energy, E, but do calculate the potential energy, U. The equation above should be recast as

$$\langle T \rangle = \left[\frac{\langle (U - \langle U \rangle)^2 \rangle}{3(N-1)k_{\mathrm{B}}c_{v,U}} \right]^{1/2}.$$

The total specific heat is the sum of $c_{v,U}$ (the contribution from the potential energy) and the contribution from the kinetic energy, $c_{v,K}$:

$$c_v = c_{v,U} + c_{v,K}.$$

On a per atom basis, the value of $c_{v,K}$ is $1.5k_{\mathrm{B}}$, independent of temperature.