24-623/12-623 2015 HW#6

Total points: 40
Assigned: November 9, 2015.
Due: November 27, 2015, midnight to Blackboard. Please use the Blackboard discussion board to ask questions of the instructor or the other students.

1. (25 points) Modify your LJ MD code so that it can also perform Metropolis MC NVT simulations. Then, using the 256-atom liquid LJ system provided in HW#3:

(a) Determine $\langle U \rangle$ (dimensionless) and $\langle P \rangle$ (dimensional) for $L = 6.8$ and an argon temperature of 100 K. Explain how you determined the maximum trial move step size and when your system is equilibrated. Compare your answers to what you found in HW#3.

(b) Determine and plot $\langle P \rangle$ (dimensional) 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. Compare your answer to what you found in HW#4.

2. (15 points) The thermodynamic temperature in the NVT ensemble is given by

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

Recall that $3c_v$ is the heat capacity per atom.

In MC simulation, you don't calculate the total energy, E, but do calculate the potential energy, U. The above equation 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 heat capacity 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.

Use the potential energy fluctuations from a Metropolis MC NVT simulation to find the total heat capacity of the LJ argon liquid at a temperature of 100 K. Report the result in J/kg-K and compare it to what you found in HW#4. Explain what you did using words, plots, tables, etc. Just giving the answer is not sufficient.

From the standpoint of computational efficiency, do you recommend using MD or MC to predict heat capacity? Why?