24-623/12-623 2017 HW#6

Total points: 50
Assigned: November 6, 2017.
Due: November 26, 2017, midnight to Canvas. Please use the Canvas discussion board to ask questions of the instructor, the course assistant, or the other students.

1. (30 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 size of the trial move and when your system is equilibrated. Compare your answers to what you predict from your NVT MD code (you may need to run additional simulations beyond what you did in HW#4).

(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. (20 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 can 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 heat capacity per atom is the sum of the contributions from the potential energy, $c_{v,U}$, and the kinetic energy, $c_{v,K}$:

$$3c_v = 3c_{v,U} + c_{v,K}.$$

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 heat capacity of the LJ argon liquid at a temperature of 100 K for $L = 7.4$. Report the result in J/kg-K and compare it to what you found in HW#4. Explain what you did. Just giving the answer is not sufficient.