ASEN6519: Molecular Simulation of Materials
Spring 2019

Homework # 4

Instructor: Sanghamitra Neogi

Assigned: March 13, 2019
Due: March 22, 2019, 11:59 PM to Canvas

Total points: 40

1. (10 points) In Homework1, 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 (*bonded and non-bonded*) 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 and particles to start.

2. (30 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 coordinates (with dimension) for a 256-atom liquid system in a cubic simulation cell of side length $\sim$22Å are available in the file liquid256.xyz on Canvas. Modify your MD code so that it:

   (i) Randomly initializes the particle velocities in a manner that gives the system zero total momentum.

   (ii) Incorporates the continuous force and continuous energy cutoff scheme with a dimensionless cutoff of 2.5.

   (iii) Calculates the instantaneous temperature.

   (iv) 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).

   I will introduce the details of the NVE ensemble in the next lecture. This problem could be solved without that knowledge for now. You will also implement the NVT ensemble later.

   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:

   (v) Time variation of kinetic energy, potential energy, total energy, and temperature for 200 units of LJ time (i.e., 100,000 time steps). The total energy should be conserved.

   (vi) Conservation of momentum in the x, y, and z directions.