PHYS 5120: homework2

NOTE: Modify "md.py" and write your own codes to do the calculations. Results from third-party packages will NOT be accepted. VMD is for visualization only. You are allowed to use the math tools, e.g., fitting, integration from Numpy. (2 pages, 5 questions)

1. Molecular dynamics simulations of Lennard-Jones argon

The experimental data for Lennard-Jones argon:

$$\epsilon/k_B = 119.8K, \sigma = 3.405\mathring{A}, M = 0.03994kg/mol \tag{1}$$

Use the "md.py" code provided here to run a MD simulation at the temperature $T = 202$ K and the density $\rho = 1460$ kg/m^3. The simulation time after equilibrium should be at least 12 picoseconds.

1. Calculate the temperature and the number density in reduced units.
2. Choose a proper time step. Plot kinetic energy, potential energy, and total energy versus simulation time. Are they stable?
3. Output unfolded coordinates as well as velocities in the Gromacs gro format: `http://manual.gromacs.org/archive/5.0.3/online/gro.html`. The length unit is nanometer (nm); the time unit is picosecond (ps); the velocity unit is nm/ps. A sample gro file for a MD trajectory is provided here. Save the trajectory on your machine (NOT canvas.ust.hk) and visualize it using the VMD software: `http://www.ks.uiuc.edu/Research/vmd/`. In VMD, choose CPK as the drawing method (Graphics -> Representations -> Drawing Method) Attach *one* VMD screen shot in your PDF report. If your time step is very small, you do not need to write down every MD step, why?
   Use the saved gro file to do the following analyses.
4. Write your own code to plot the radial distribution function of argon.

5. Calculate the diffusion constant (coefficient) using both the Einstein relation [1] and the Green-Kubo method. Are the two results consistent? Because of periodic boundary conditions, we have folded and unfolded coordinates. Which one should be used to calculate the mean squared displacement? Why?

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[1] To calculate the mean squared displacement, you may also vary the starting point $t = 0$, just like in the auto-correlation function. Here, you can use only one starting point to simplify the calculation.