12 March 2020

Question 1: LAMMPS Simulation of Argon and Water (NPT)

Using the trajectory generated in class (make sure to have nsteps = 1000000 and dump every 1000 steps), report the following analysis in form of plots:
a) Radial distribution function
b) Temperature vs time
c) Potential, kinetic and total energy vs time

d) Calculate specific heat of the system. (specific heat = variance of energy/k(T*T))

Question 2: GROMACS Simulation of Alanine-dipeptide and Lysozyme

a) Plot phi-psi angles
1) From a 1 ns trajectory and compare with 10 ns trajectory
2) From a simulation at T=310K and compare with other at T=600K (see if you are able to simulate at T=600K).

Question 3: Write a general code for RDF calculation.

Please note the date of submission is 24th March 2020.