Simulation of Lennard-Jones spheres – writing your own LAMMPS scripts and executing

Your mid-term project is an exercise in Setting up a MD Simulation using LAMMPS. You should be able to do this if you follow the tutorials, LAMMPS manual and the lectures. Specifically, the project involves simulating a Lennard-Jones (LJ) sphere based problem and calculating some static properties.

Submission: The project must be carried out individually according to the problem assigned. The submission will be in the following form,

i. Brief overview about the understanding of the problem and your approach

ii. LAMMPS input script

iii. Sample output trajectory

iv. A properly labelled plot as asked in the particular problem.

Be realistic with the size of the simulation box and number of particles according to the computational power of your laptop/PC. You need to carefully model your problem, write a logical Lammps script, and carry out the simulation to the desired state.

Problem 1	Problem 2	Problem 3	Problem 4
[redacted]	[redacted]	[redacted]	[redacted]
	Shahid Ahmed		
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Problem-2 Adsorption

Consider a collection of two types of spheres, one of type-1(adsorbent) and N numbers of type-2(adsorbate) in a cubic box of length, L, such that the adsorbent is situated at the centre of the box and type-2 spheres occupy the volume with density 0.6. The spheres interact with each other in a pair-wise manner only via LJ interactions. Thus, LJ interactions are the only contributions to the internal energy of the system. Assume the following,

i. LJ parameters, $\varepsilon_{LJ(1\text{-}1)}$ = 0.1, $\varepsilon_{LJ(2\text{-}2)}$ = 1.0, $\varepsilon_{LJ(1\text{-}2)}$ = 1.5, $\sigma_{LJ(\text{Type-}1)}$ = 4.0, $\sigma_{LJ(\text{Type-}2)}$ = 1.0, $r_c = 2.5\sigma$

ii. periodic boundary conditions

iii. Constant N, V, and E.

You should have all the box boundaries set to periodic. Carry out the simulation till the equilibrium with an appropriate time step. Choose an appropriate size of the simulation box to avoid any overlapping. Make sure the adsorbent does not move from its position.

You may use any programming platform/ language, if required anywhere.

a. Generate output files corresponding to the phase space trajectory of the system; i.e., positions and velocities as functions of time

b. Calculate the radial distribution function (rdf) at different timesteps to quantify the adsorption of particles. Plot the rdf for the system of LJ spheres and compare your results with those from either books or literature.

c. Calculate the average surface area covered by the smaller spheres due to adsorption on the bigger sphere.