MM 722 **Assignment 2**

1. ***Atomic trajectories in a confined volume***: Imagine N molecules of an ideal gas confined inside a 3-dimensional cubical volume, V, at a temperature T. An imaginary partition between the box defines the left and right halves of the box. If n is the number of molecules in the LHS of the box and n' is the number of molecules in the RHS of the box, conservation implies that,

$$n + n' = N$$

Consider a gas of N particles where $N = 4$. You are provided the time evolution data for this system in the form of a LAMMPS dump file in your folders. The files are named as "dump_*N.*file", where N is the number of particles in the volume. Calculate the following,

a. Plot the trajectory of Atom id 1 as a function of time along the *x-, y-,* and *z-* directions respectively. You will have three plots in form of *x vs t, y vs t* and *z vs t.*

b. We should be able to calculate n and n' for each frame from the dump (output) file. On the same plot, show the variations of n and n' as functions of time (*or number of frames*). What is your observation?

c. What is basis of estimation of the two quantities n and n'? In other words, which plane would you use to define the *left* and *right* halves of the box? Use a plot to prove that any of the three planes, $X = L/2$, $Y = L/2$, $Z = L/2$ can be used.

NOTE: The dump files contain information in the following manner. Each snapshot is represented by (N+9) lines. The first nine lines constitute the header for each snapshot and provide information about the box dimensions and the timestep number. The next N lines have coordinate information for all the coordinates. Each line has five column,

1. Atom id
2. Atom type (all atoms are of the same type for this problem)
3. Atom x-coordinate
4. Atom y-coordinate
5. Atom z-coordinate