Diffusion Constant Calculation: In class we have learnt how to calculate the self-diffusivity from MD data. In today's assignment, we want to simulate the dynamics of water and evaluate the diffusivity of water at room temperature. Experimentally measured values of water self-diffusivity are approximately $2.34 \pm 0.05 \times 10^{-9}$ m^2/sec at 298 K and 1 atm pressure.

In this simulation 116 water molecules are confined in a box of size $16 \times 16 \times 16$ $Å^3$ with periodic boundary conditions. The simulations are carried under NVE conditions, with a Langevin thermostat to maintain temperature at 298 K and a Berendsen barostat to maintain the pressure at 1 atm pressure (Note: The barostat will not do a good job and the fluctuations will be very large, mainly due to the small system size).

Each water molecule is represented by a three-site water model called the TIP3P, where each site represents the three atoms that make up the water molecule, namely, two hydrogens and one oxygen. Each site is ascribed a point charge, -0.834 for the oxygen site and +0.417 for each of the two hydrogen sites, thus making every molecule electrically neutral. Lennard-Jones parameters are also defined for both oxygen and hydrogen atoms.

1. Zero the linear momentum before the simulation starts.

2. You have to run the MD code for a desired amount of time, may be 200 ps, and calculate the self -diffusion coefficient of water from the position coordinate data.

3. Make appropriate changes to the script to run the same simulation in a NVE ensemble without any temperature or pressure controls. Calculate the diffusion constant based on this simulation.

4. Next, run the same simulation in a NVT ensemble using a Nose-Hoover thermostat for temperature control. Again, calculate diffusion constant for this ensemble.

The initial run corresponds to an equilibration step with a timestep of 0.5 fs for a duration of 1ps (2000 steps), and the data is written in a file called "*equilibrate.dump*". The second step or the production run corresponds to a timestep of 1 fs and the duration of the run has to be decided by you. The output is written to a file called "*solvate.dump*".

<u>*Calculation of the diffusion constant*</u> You need to calculate the diffusion constant using two methods,

i. Use the LAMMPS compute, compute msd, to calculate the diffusion constant.
ii. Write a post-processing script/ program to calculate the diffusion contant from the trajectory output in the dump file. You can use the oxygen atom positions to define the position of a water molecule.

Question to ponder: On what physical basis will you estimate a duration for the production run?