CH504 - Computational Chemistry
Lab Assignment 2

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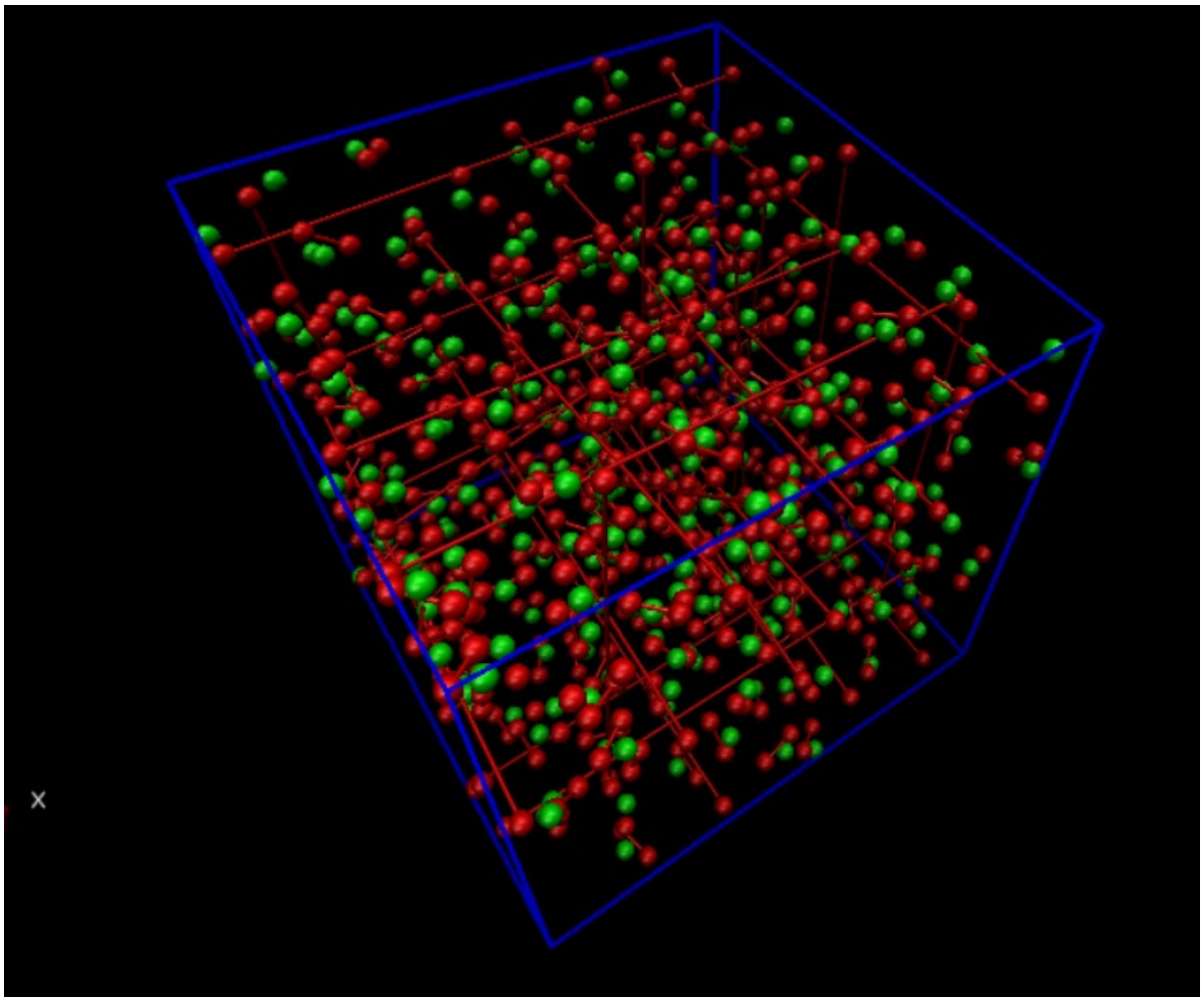
April 8, 2023

Objective:

- To use the LAMMPS to perform a simple molecular dynamics simulation.
- Using LAMMPS, find the plots Mean square Displacement (MSD) and Radial Distribution Function (RDF). Further calculate the Mean squared displacement, diffusion coefficient and radial distribution, and loading the trajectory and generating the snapshots for the simulation functions for TIP4P water model.

Snapshot of the System:



- **colour coding:** water : red
- **Box Dimensions:** $30 \times 30 \times 30$ (that is a cube with side length 30σ)
- **Periodic Boundary Conditions:** periodic boundary conditions for all dimensions

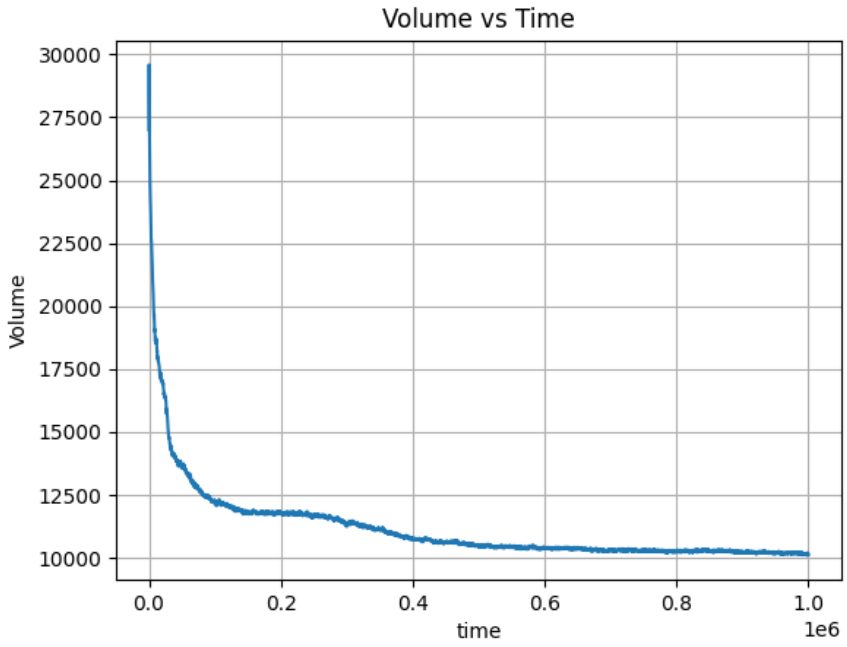
List of all the Parameters used for the simulations

1. **Box Dimensions:** $30 \times 30 \times 30$
2. **Interaction Parameter:** As per TIP4P model
3. **Number of Particles:** H: 600, O: 300
4. **Timestep:** 2
5. **Simulation Length:** $5 * 10^5$ runs for equillibrium and 10^6 runs for production

```
pair_style       lj/cut/tip4p/cut 1 2 1 1 0.1577 10.0 8.5

pair_coeff       1 1  0.21084  3.1668

pair_coeff       2 2  0.0     0.0

pair_coeff       1 2  0.0     0.0
```

Plot for Volume

Note: For all the plots we have 300 oxygen atoms and 600 hydrogen atoms

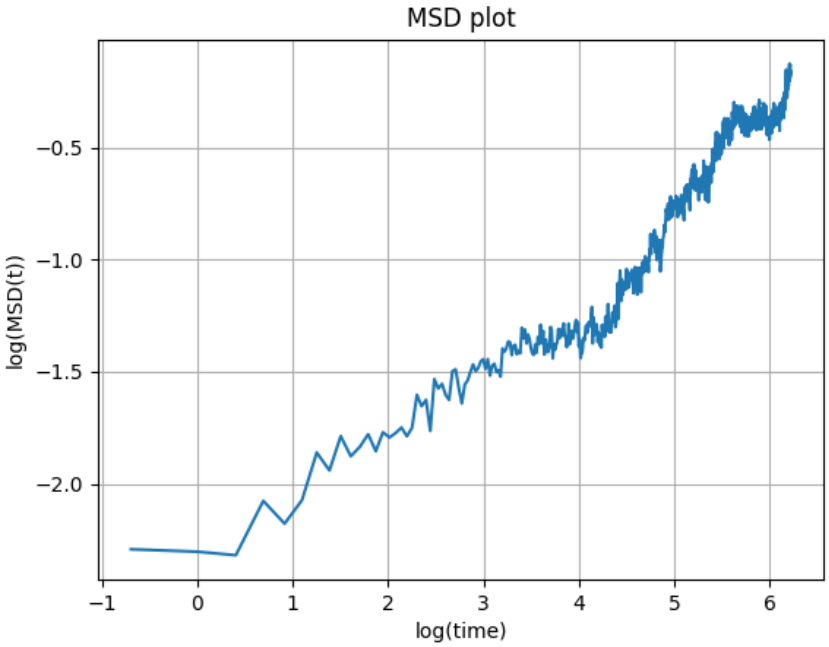


Final Volume = 10120.213
Final Box Dimension (size length = $(FinalVolume)^{\frac{1}{3}}$) = 21.629*21.629*21.629

Observation

We can see from the plot above that the volume is continuously decreasing with time. This is because of the condensation of water caused by decreasing temperature with time.

Plots for MSDs

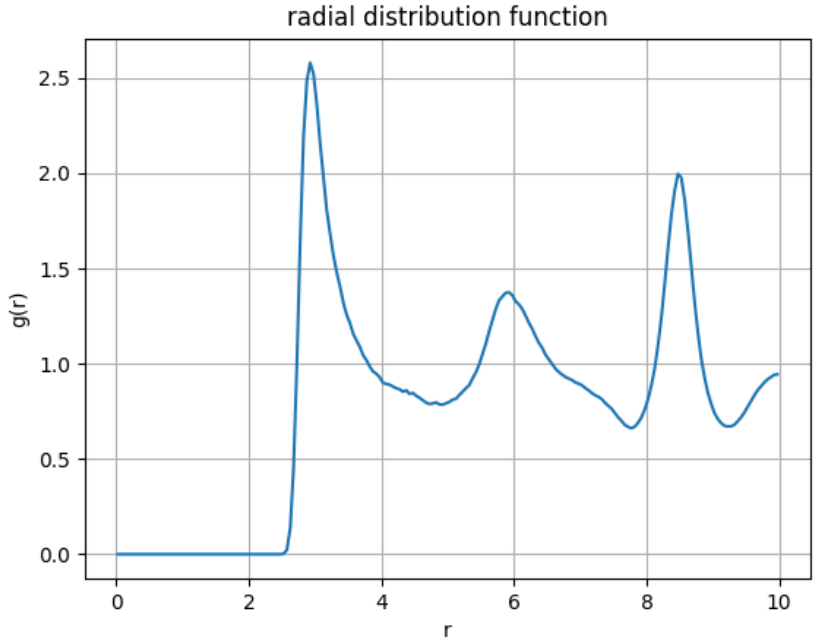


Since the plot for average displacement is a straight line, so is the plot on log-log scale. This can be expected as $\log(MSD) \approx \log(6D) + \log(t)$ for large enough values of t. The straight line might not perfectly fit the given plot but still it would be a good approximation for this case. One can also observe a lot of noise near larger values of t which is probably because we plotted on log-log scale, so a lot of data points are close to each other, therefore giving it noise like appearance. But overall the results generated satisfy the diffusion equation.

Calculations

For Oxygen
Intercept = -11.185178564418253
antilog(Intercept) = 1.3878376668862493e-05
D = antilog(Intercept)/6 = 2.313062778143749e-06

Plot for RDF



Observation

One can see that the first minimum is between 3 and 4, around 3.5. This is somewhat similar to online data available through X-ray scattering.