CH504 - Computational Chemistry
Lab Assignment 1

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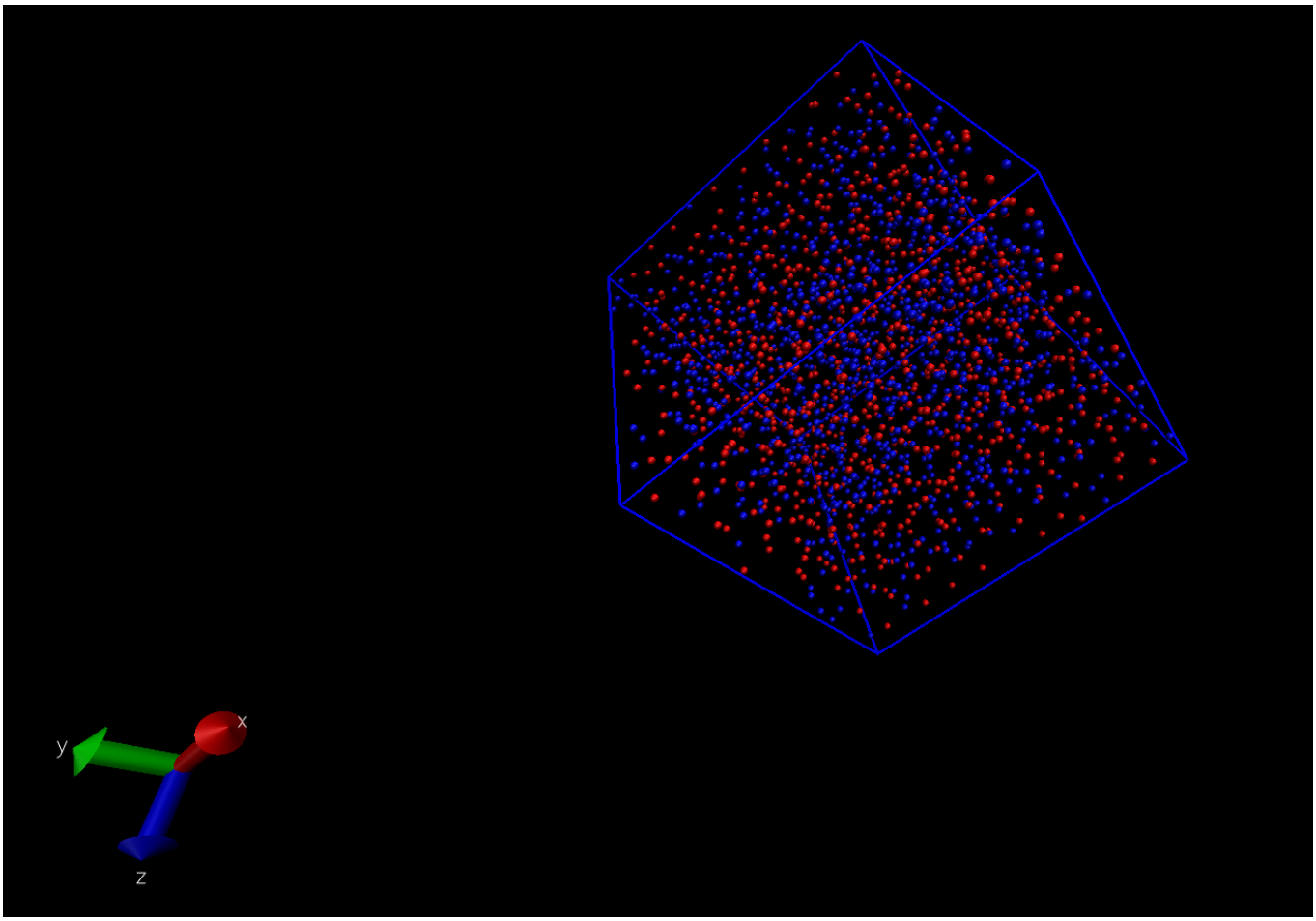
Objective:

- To use the LAMMPS to perform a simple molecular dynamics simulation of a binary fluid. The system we use for this tutorial is called Lennard-Jones fluid.
- Using LAMMPS, find the plots for potential, total, kinetic energies of the system. Further calculate the Mean squared displacement, diffusion coefficient and radial distribution, and loading the trajectory and generating the snapshots for the simulation. functions for both the particles.

Snapshot of the System:



- **colour coding:** Type A: Blue, Type B: Red
- **Box Dimensions:** $40 \times 40 \times 40$ (that is a cube with side length 40σ)
- **Periodic Boundary Conditions:** periodic boundary conditions for all dimensions

List of all the Parameters used for the simulations

1. **Box Dimensions:** $40 \times 40 \times 40$
2. **Interaction Parameter:** $\epsilon = 2$
3. **Number of Particles:** Type A: 2σ, Type B: 4σ
4. **Timestep:** 0.005
5. **Simulation Length:** 10^4 runs for equillibrium and 10^6 runs for production

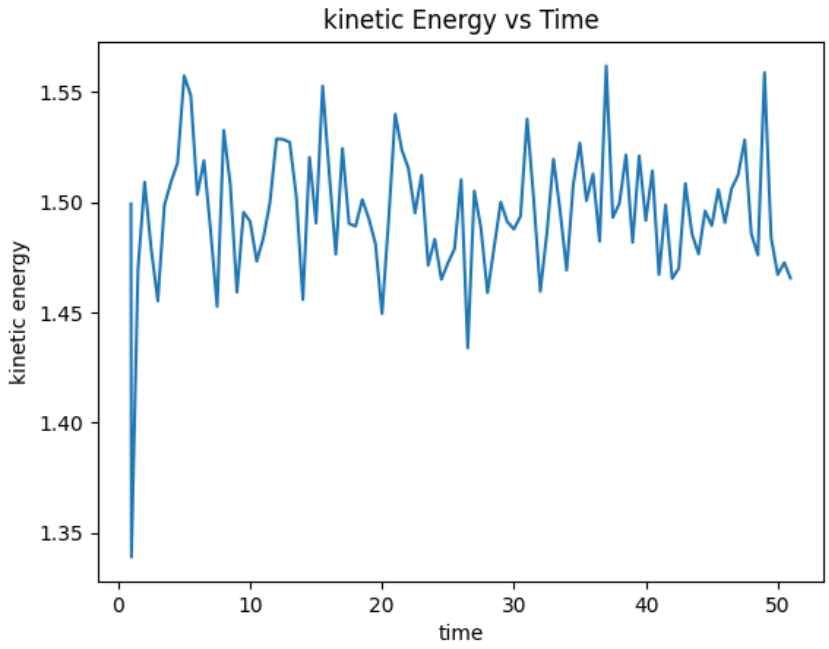
```
units           lj
dimension       3
atom_style      atomic
boundary        p p p
```

```
pair_style      lj/cut 1.12246204831
pair_coeff      1 1 2.0 2.0 2.24490409662
pair_coeff      2 2 2.0 4.0 4.489884819324
pair_coeff      1 2 2.0 3.0  3.36735614493
```

Plots for Energies

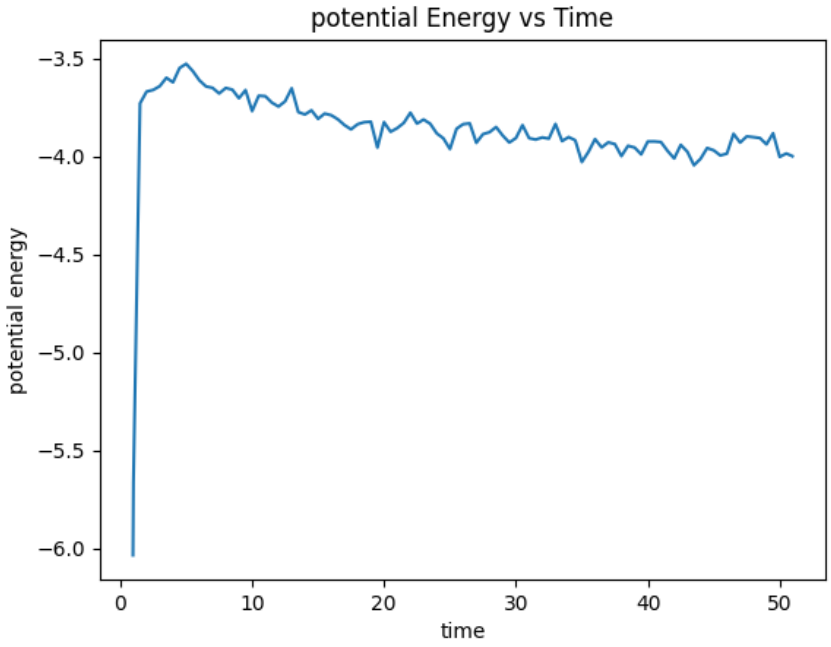
Note: for all the plots below number of particles of type A are 1200 and number of particles of type B are 1000.

Kinetic Energy



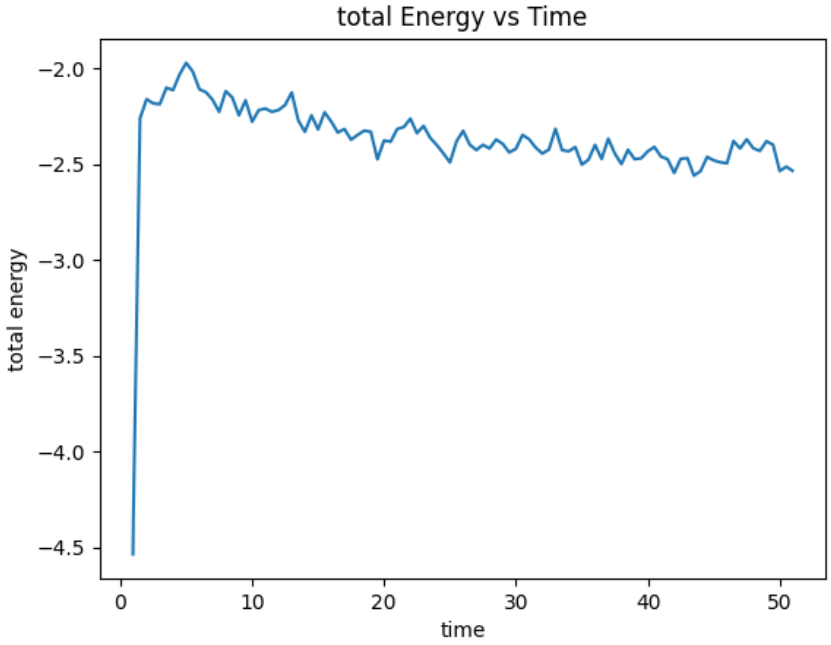
Average Kinetic Energy = 1.4952027274509805
One can observe that the kinetic energy keeps oscillating around the value 1.5 but doesn't change much because average speed of the particle does not depend on time but depends on temperature which was fixed in this case.

Potential Energy



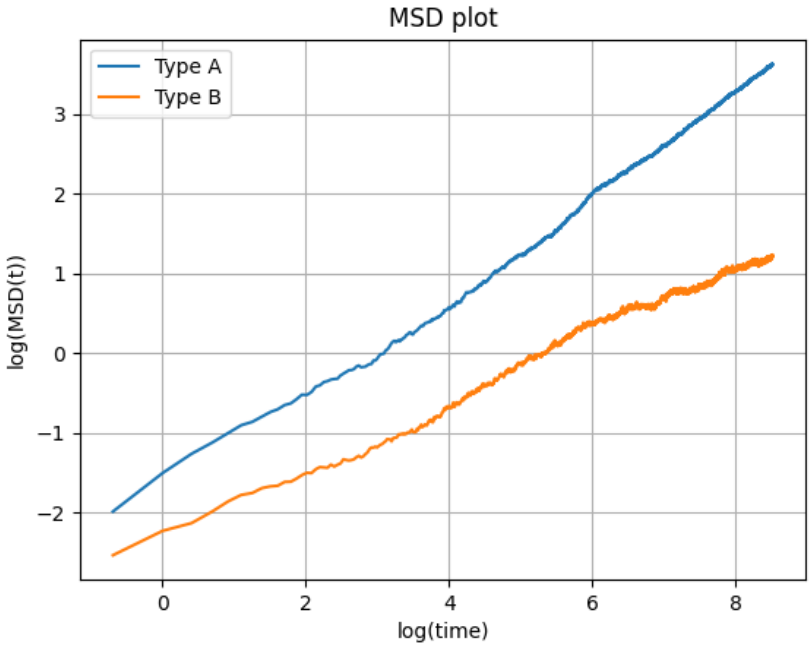
Average Potential Energy = -3.881800199019608
With time we can clearly see that the potential energy is decreasing with time. This is because in the system, interaction occurs in such a way that it acquires stability. Otherwise, over the whole period of experiment, the potential energy value remains close to little above -4.0.

Total Energy



Average Total Energy = -2.386597483333333
We can see that total energy decrases with time but remains close to little above -2.5. This is because of the fact that total energy is the sum of potential energy and kinetic energy, just like potential energy its value also decreases with time

Plots for MSDs



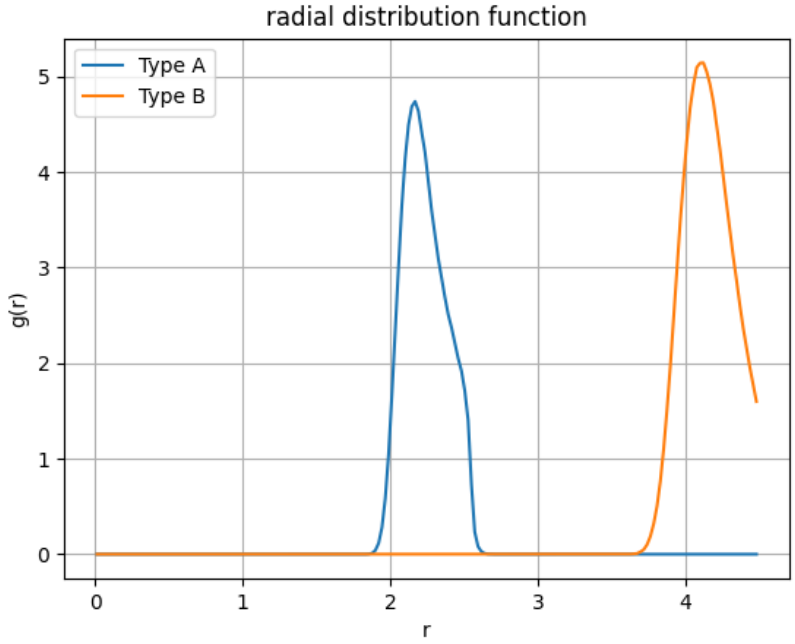
Since the plot for average displacement is a straight line, so is the plot on log-log scale. This can be expected as $\log(MSD) \approx \log(6D) + \log(t)$ for large enough values of t. One can also observe a lot of noise near larger values of t which is probably because we plotted on log-log scale, 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 particle 1
Intercept = -4.559176953772244
antilog(Intercept) = 0.010470673246073113
D = antilog(Intercept)/6 = 0.0017451122076788522

For particle 2
Intercept = -6.657568786092475
antilog(Intercept) = 0.001284264900628431
D = antilog(Intercept)/6 = 0.0002140441501047385

Plot for RDF



Observation

Observe that rdf plots for both the particles have peak at certain value of radius r. The maxima for Type A particles are close to 2 and similarly the maxima for Type B particles are close to 4 which implies from the fact that we have set the size of the particles to 2σ and 4σ respectively.