CH504 - Computational Chemistry
Lab Assignment 3

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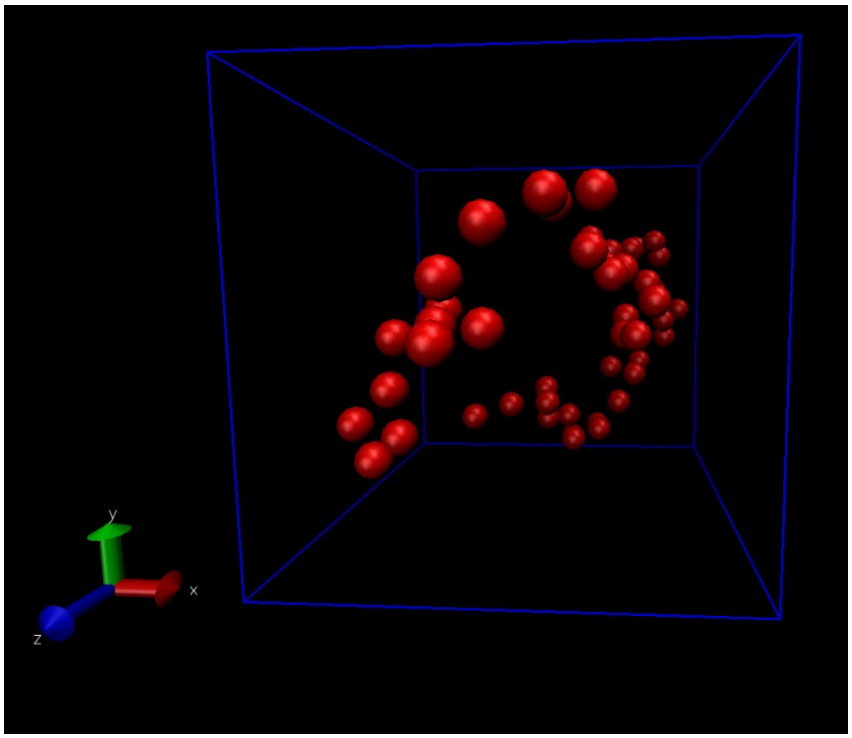
Objective:

- To simulate and analyze the bead-spring polymer chain in good solvent. The simulation box is cubic with periodic boundary conditions
- Also to plot various quantities such as energies, MSD of center of mass, MSD of central atom of the polymer and radius of gyration in both good as well as bad solvent

Snapshot of the System:



- **colour coding:** monomer : red
- **Periodic Boundary Conditions:** periodic boundary conditions for all dimensions
- Number of monomers is 50 for all the results and plots

List of all the Parameters used for the simulations

1. **Size of monomer** 1σ
2. **Interaction parameter:** 1 (good solvent), 4 (bad solvent)
3. **Timestep:** 0.001
4. **Equillibrium runs:** 10000
5. **Production runs:** 1000000

```
pair_style  lj/cut 1.12
pair_coeff  1 1 1 1 1.12
```

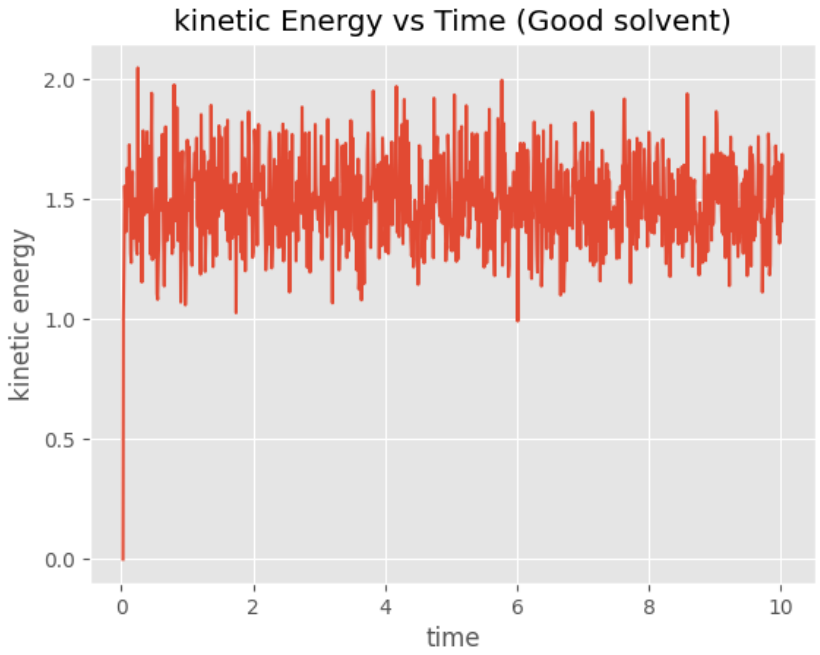
This is for the good solvent

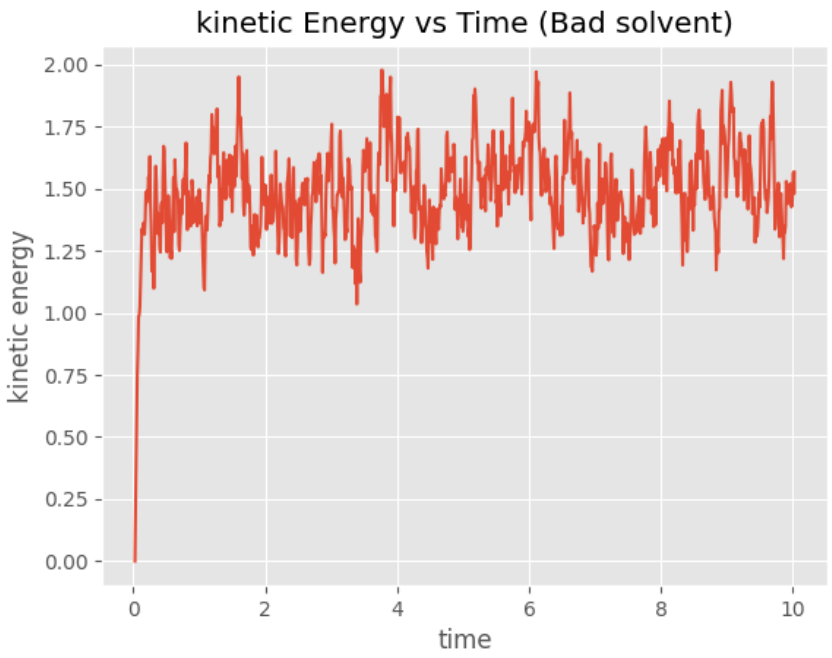
```
pair_style  lj/cut 1.12
pair_coeff  1 1 4 1 1.12
```

This is for bad solvent

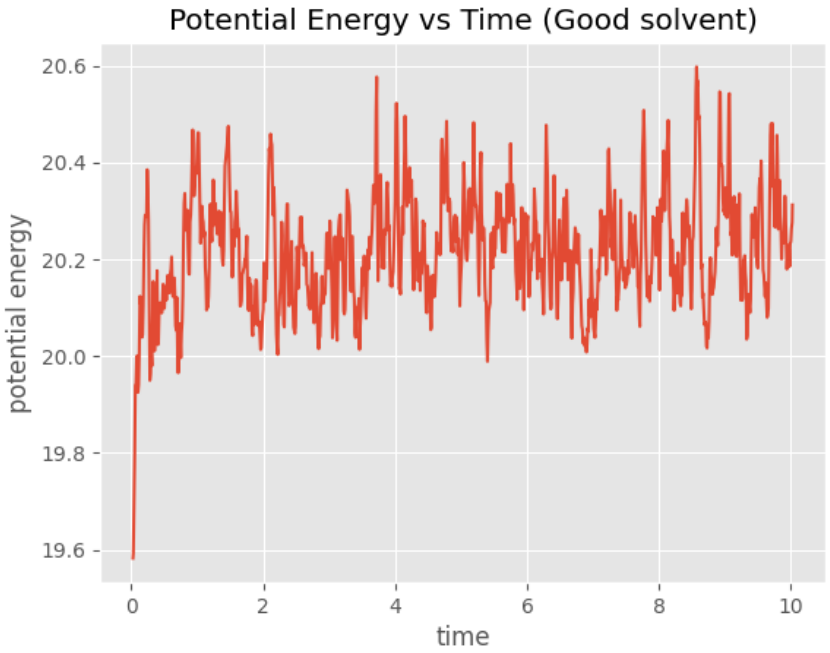
Plots for Energies

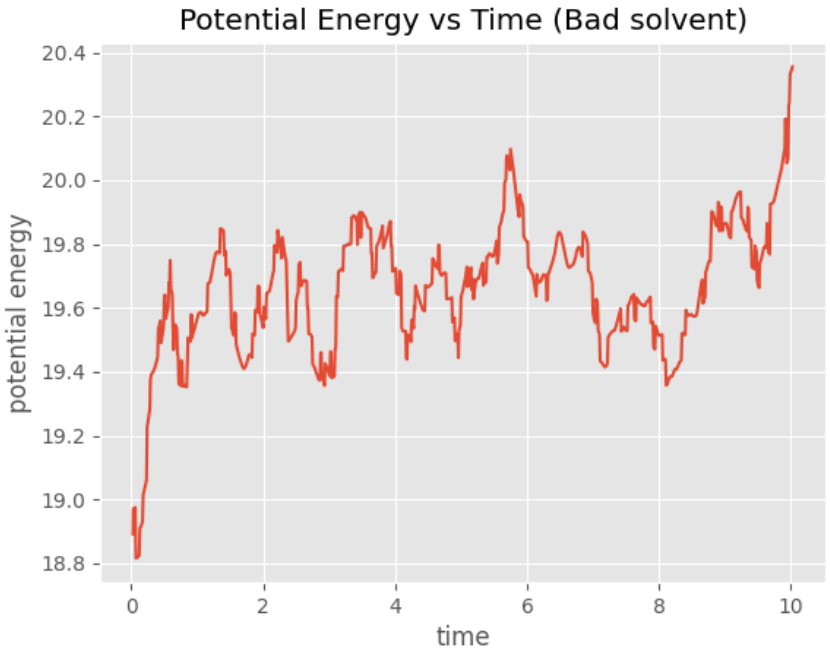
Plot for Kinetic Energies



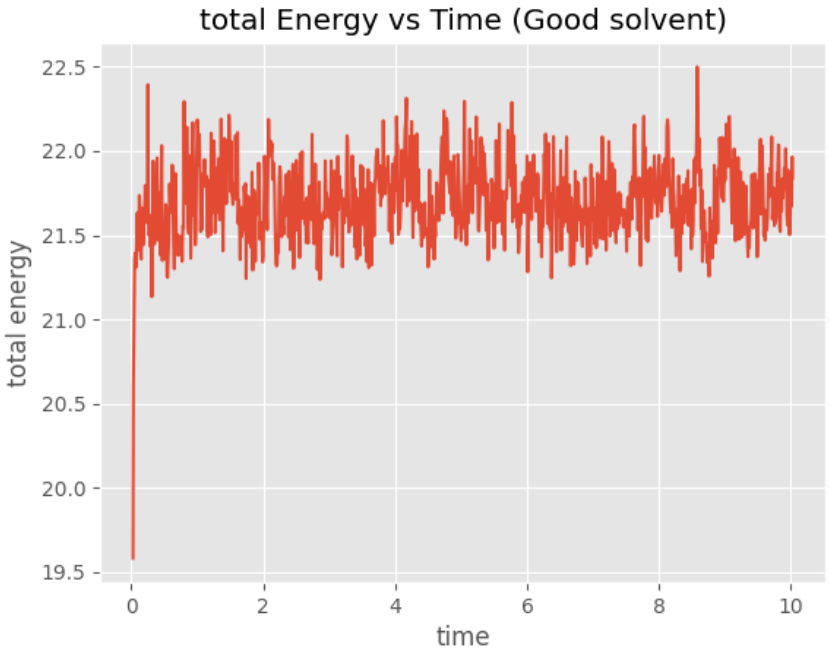

kinetic Energy vs Time (Bad solvent)
kinetic energy
time
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0
2
4
6
8
10

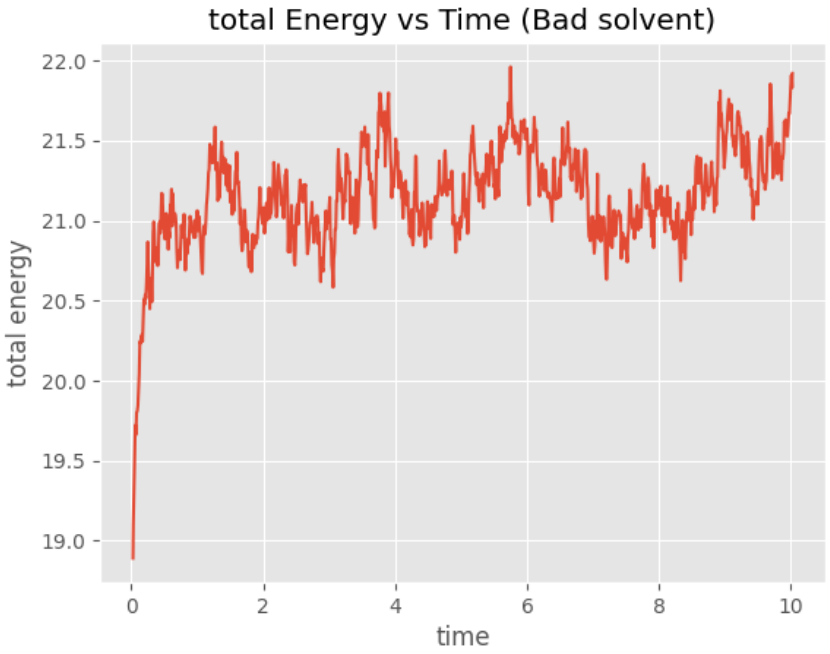
Plot for Potential Energies





Plot for Total Energies





Good Solvent

- **Average KE:** 1.4888959251497005
- **Average PE:** 20.216480080838323
- **Average TE:** 21.705376005988025

Bad Solvent

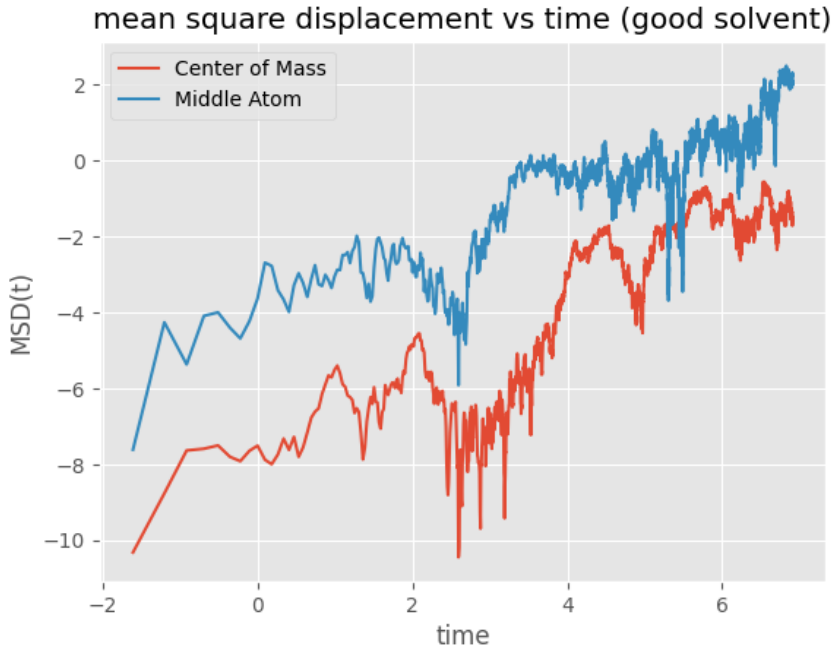
- **Average KE:** 1.4944800568862275
- **Average PE:** 19.65822805988024

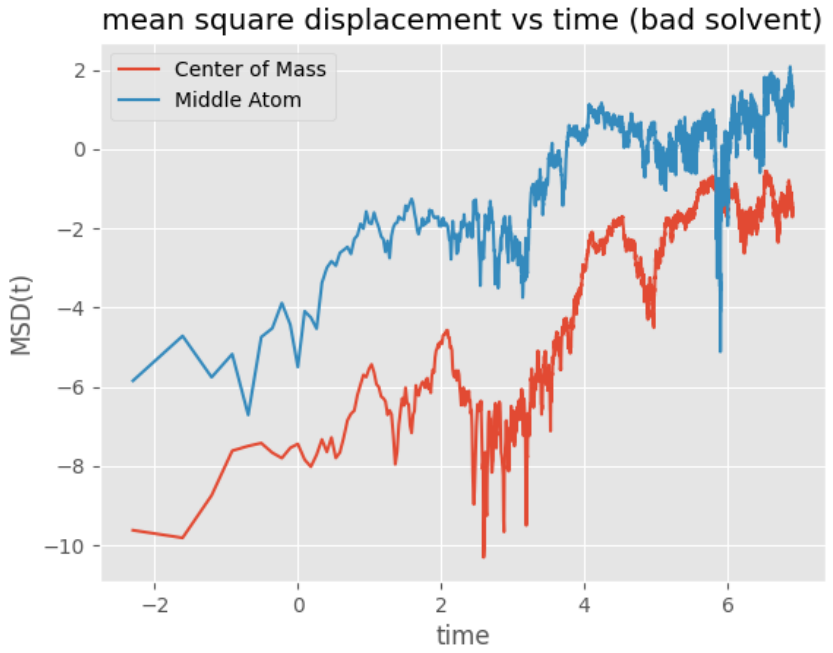
- **Average TE:** 21.15270811676647

Observation:

The value of kinetic energy is smaller in comparison to Potential energy in both the solvent. The value of total energy is close to 21.5. PE is close to 20 in both the cases (good and bad solvent). This means that movement is restricted for polymers. Also, polymer has higher kinetic energy in case of bad solvent.

Plots for MSDs



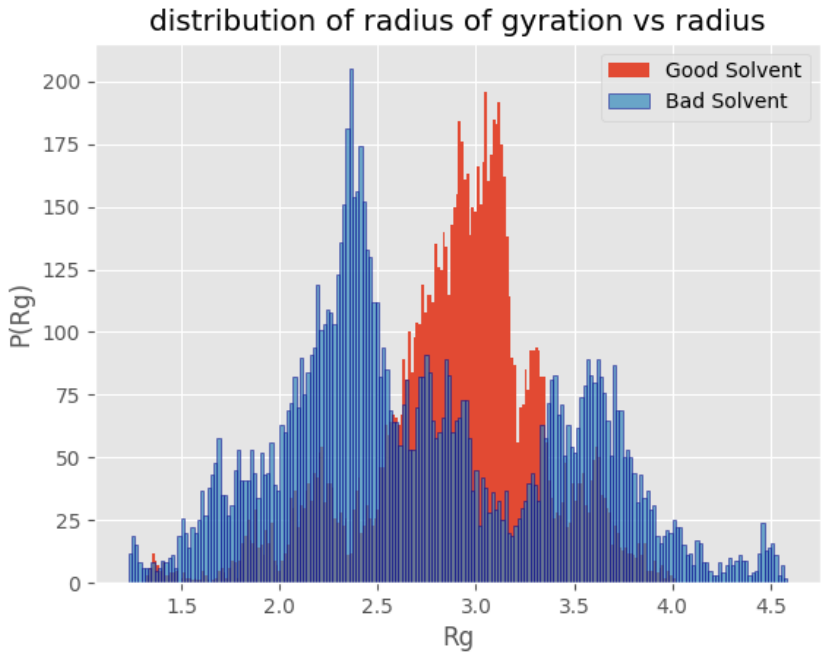


Note: The plot is generated for log scale for both the solvents.

Observation:

The overall trend of variation of log(MSD) with log(time) is linear in with noise at each point which is expected. The trend for both the solvents is almost similar. The MSD for central atom is higher than the center of mass for both solvent.

Radius of gyration



Observation

We can observe that peak probability distribution of radius of gyration in bad solvent is smaller than that for good solvent. This may be due to the fact that the polymer forms a globular structure which forces the atoms to be closer to centre of mass (And hence reduces the moment of inertia).