Molecular Dynamics study of Diffusion of Hydrophobic species in water

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Under Guidance of-
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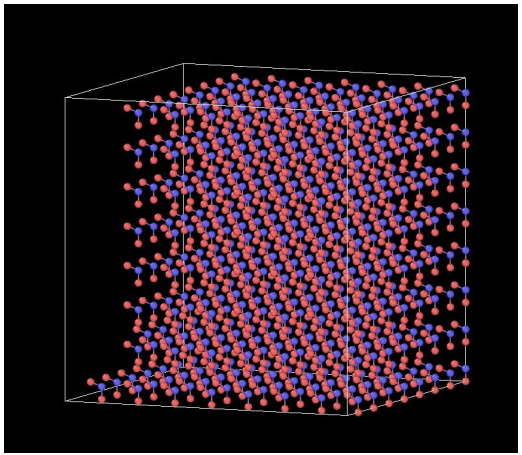
Initial System - SPC/E Water Model

- NVT Ensemble
- Dimensions of Box - 24 Armstrong
- Number of water molecules - 461
- Temperature - 315 K
- Density of water- 0.997 g/cmˆ3



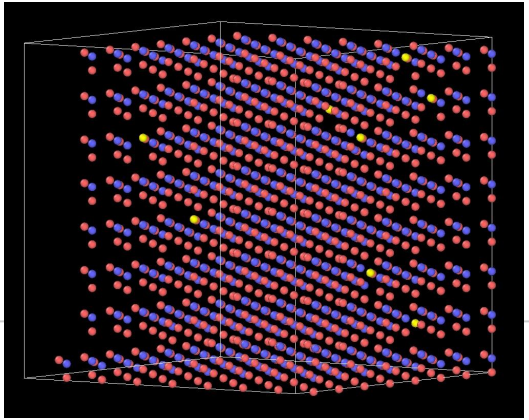
Arranged in periodic manner

Replacing 8 molecules

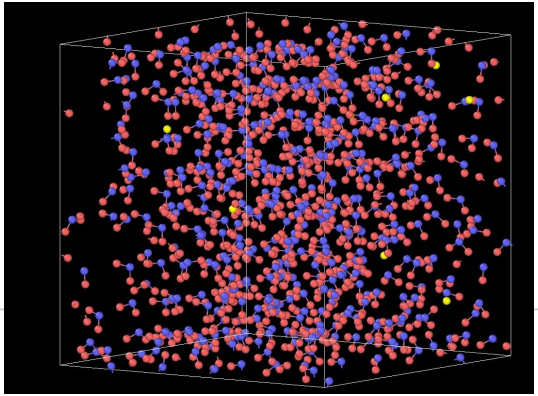
- 8 water molecules were replaced.
- 8 neutral species with different sigma (Lennard Jones Potential parameter) values were added.
- System has 453 water molecules and 8 hydrophobic species.

Simulation

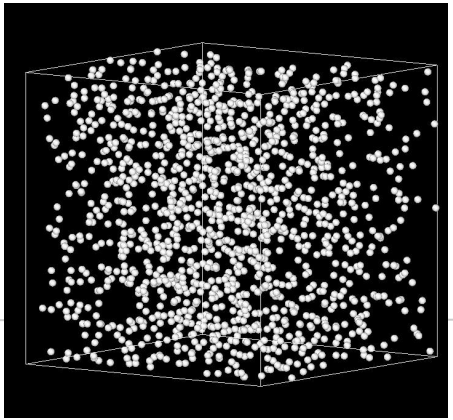
- Energy Minimization
- Thermal Equilibration of 1 ns
- Production simulation of 9 ns
- Total run of 10 ns



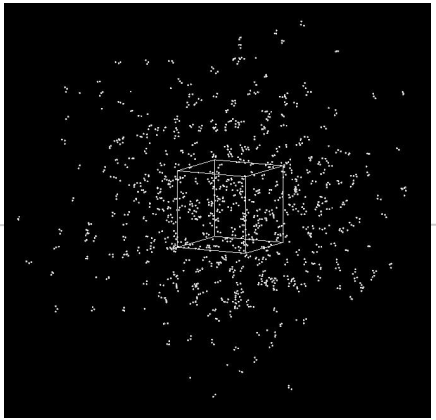
replaced
molecules initially



after minimization



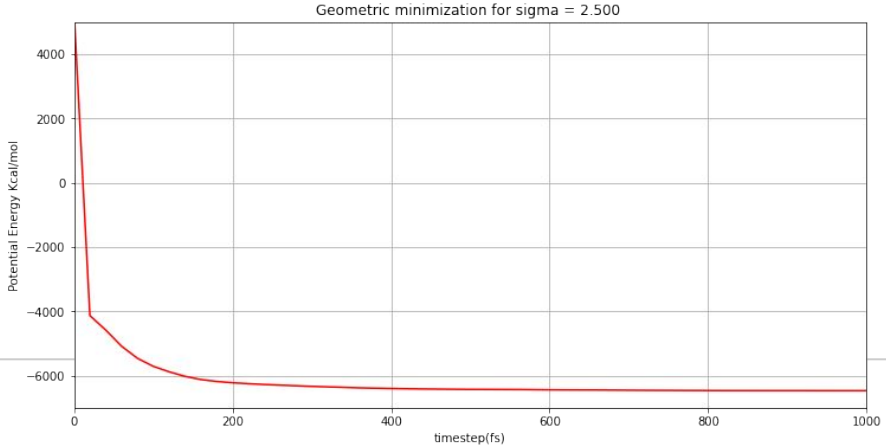
after equilibration

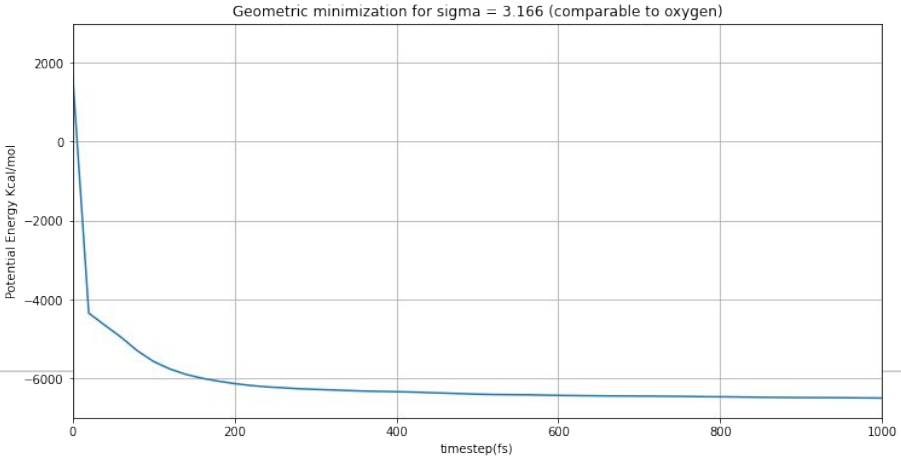


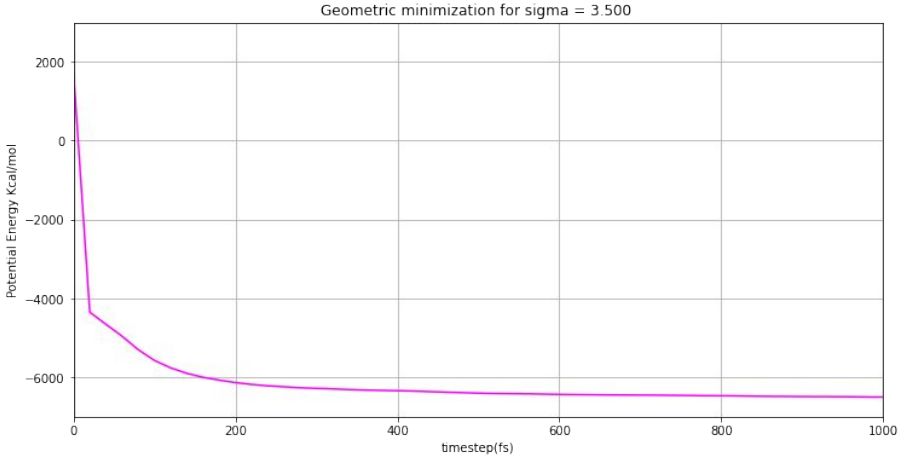
after production

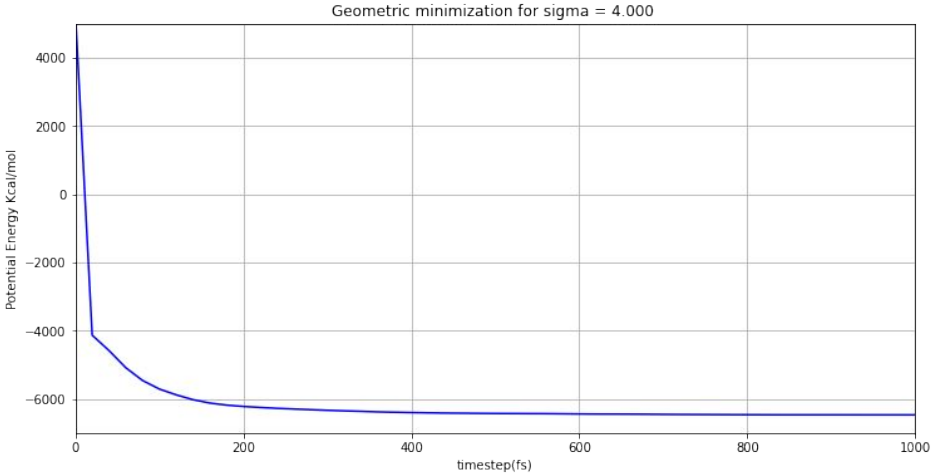
SIMULATION OF 10 NS

Minimization of Energy

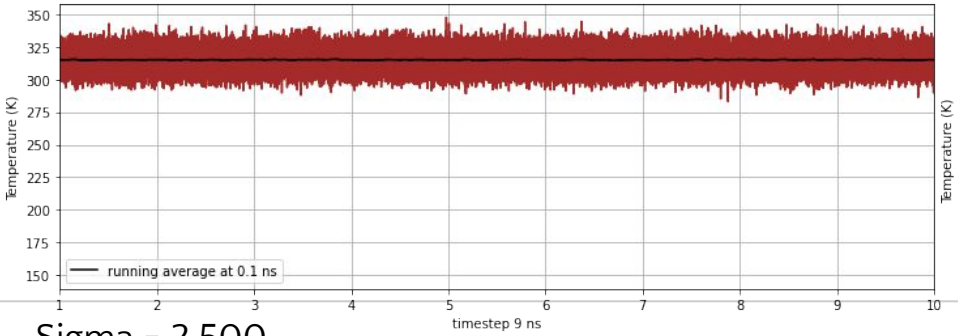




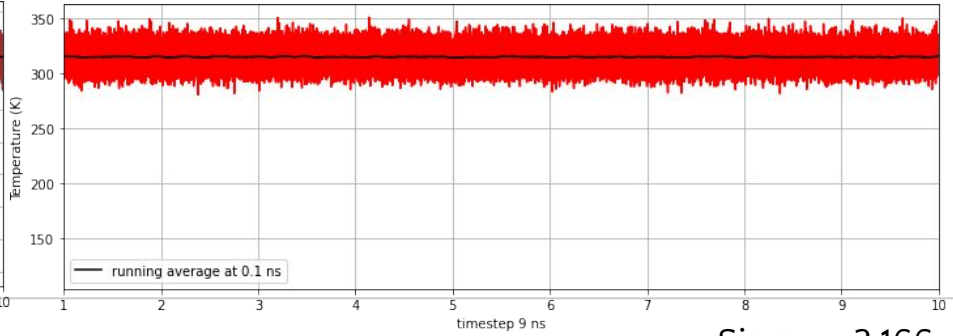




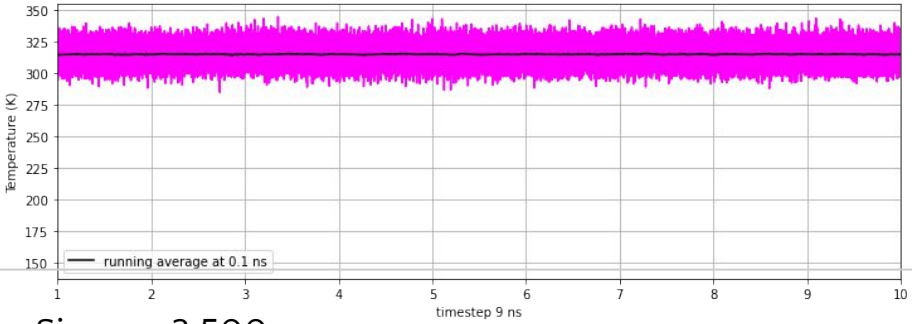
Temperature Over Time



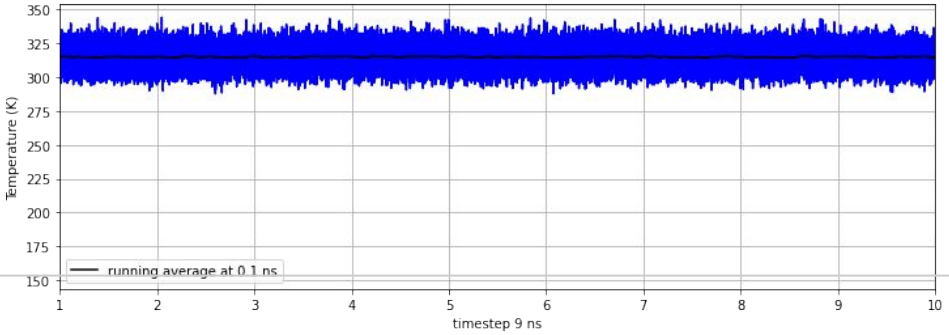
Sigma = 2.500



Sigma = 3.166



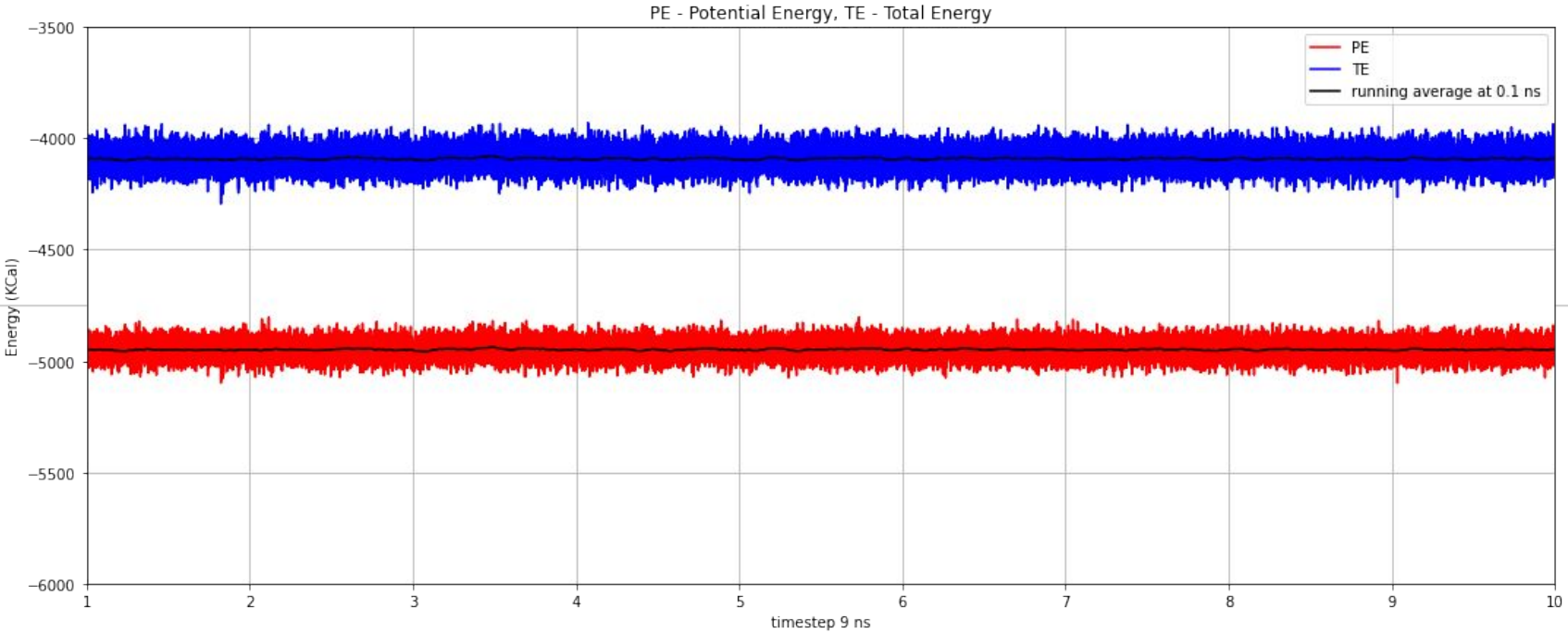
Sigma = 3.500



Sigma = 4.000

Behaviour of the temperature of the system with simulation time

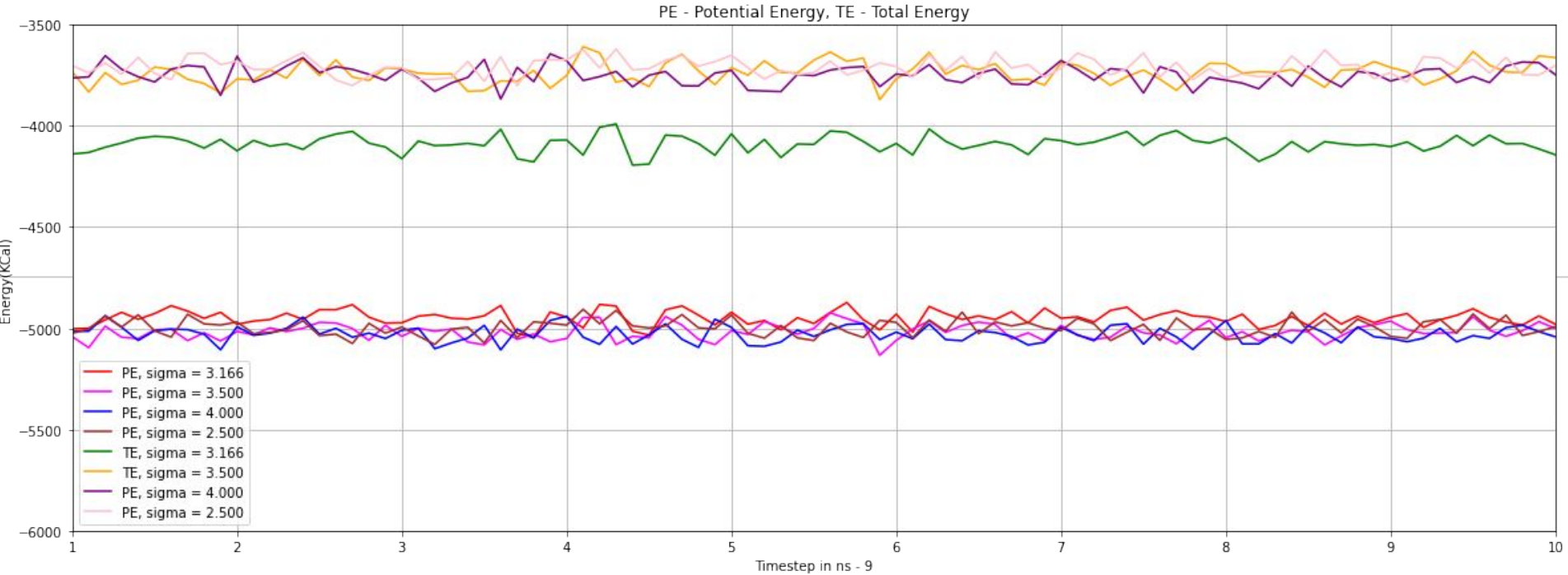
Potential Energy and Total Energy Over Time



Sigma = 3.166

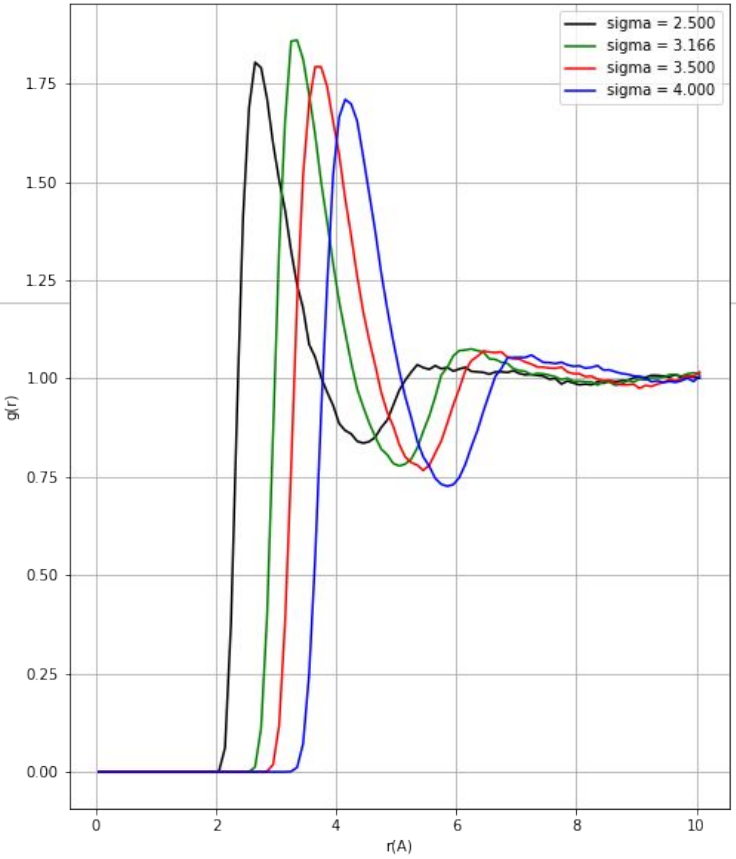
Behaviour of the Potential and Total Energy of the system over simulation time

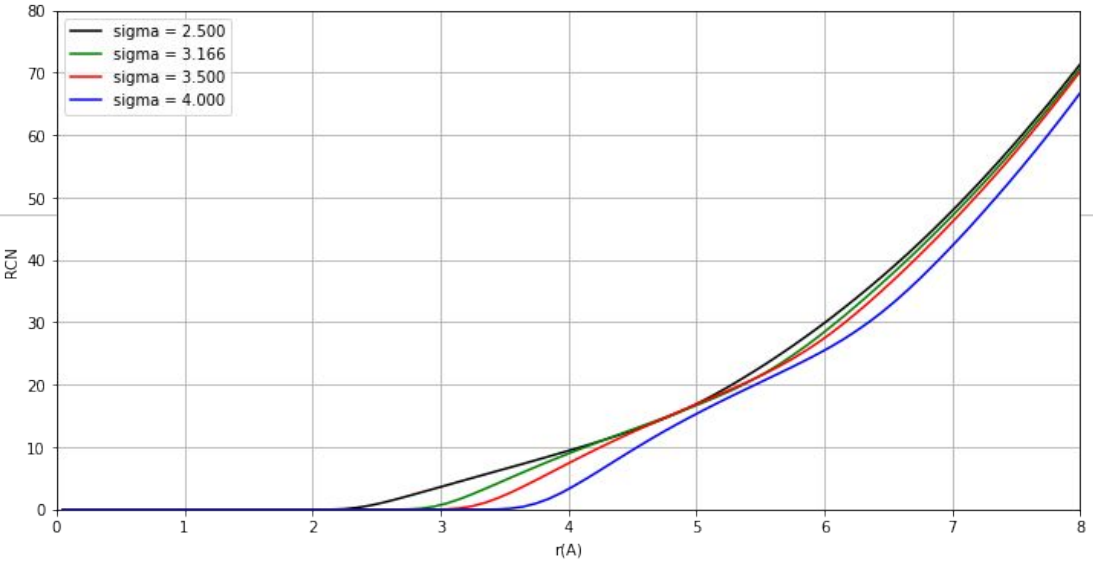
Potential Energy and Total Energy Over Time



Behaviour of the Potential and Total Energy of the system over simulation time with varying sigma values

Radial Distribution Function and Running Coordination Number





Hydrophobic Species – Oxygen RDF & RCN

RDF plot comparison from Literature

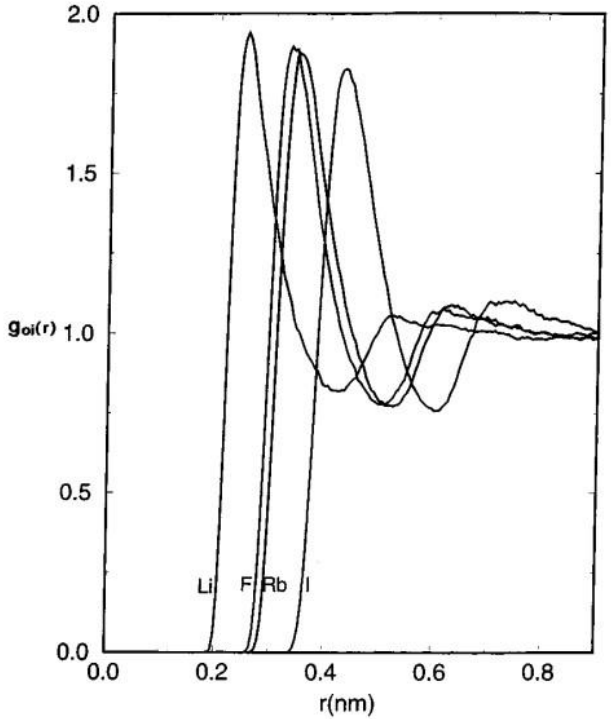
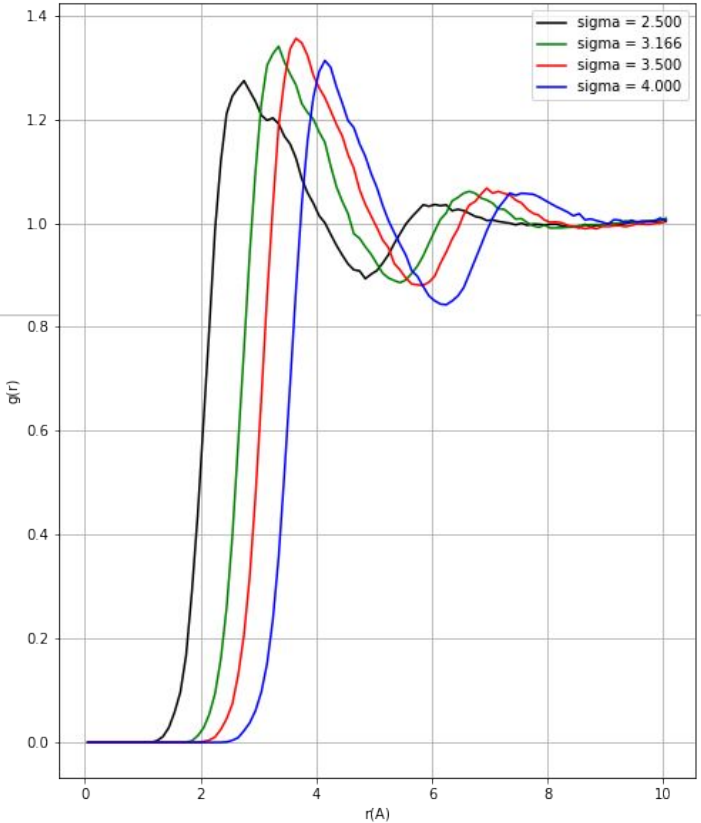
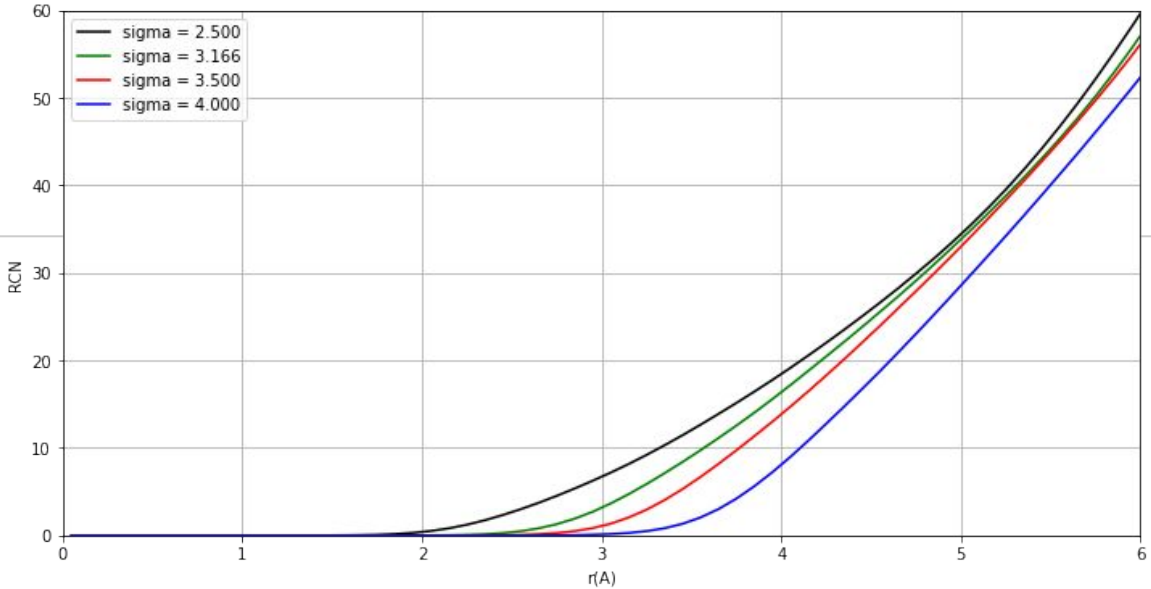


Figure 7. Solute–oxygen radial distribution functions of uncharged Li, Rb, F, and I.

Reference : Solvent Structure, Dynamics, and Ion Mobility in Aqueous Solutions at 25 °C

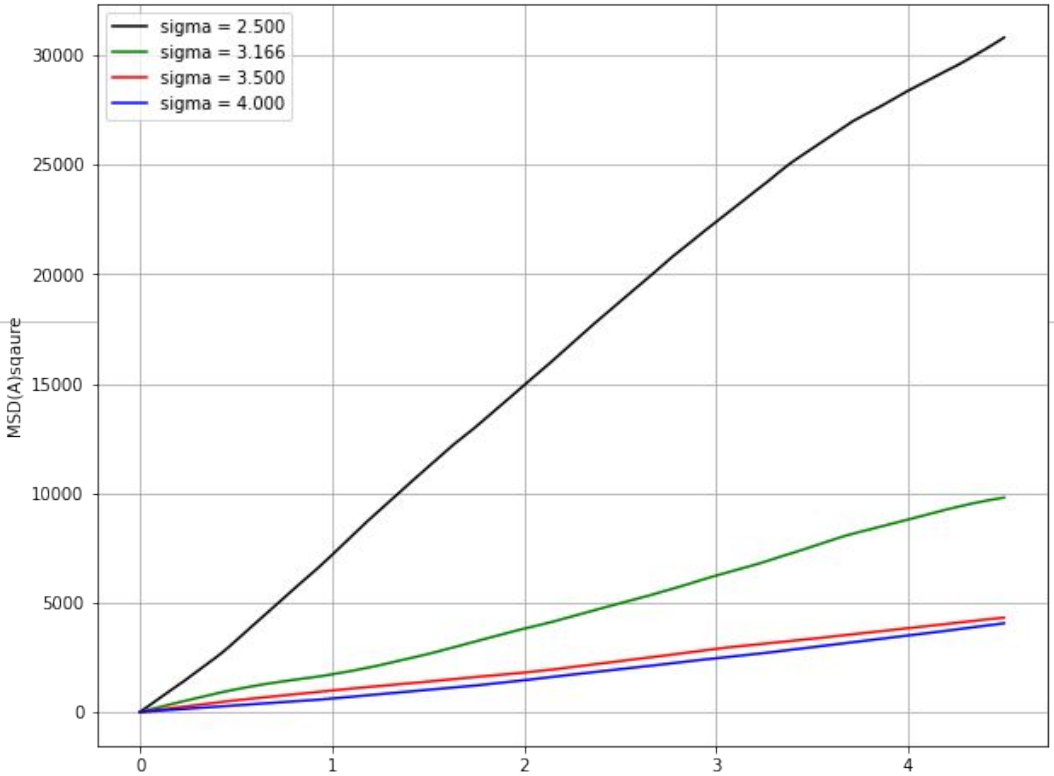
Radial Distribution Function and Running Coordination Number





Hydrophobic Species – Hydrogen RDF & RCN

Mean Square Displacement (MSD)



MSD plots for different sigma values

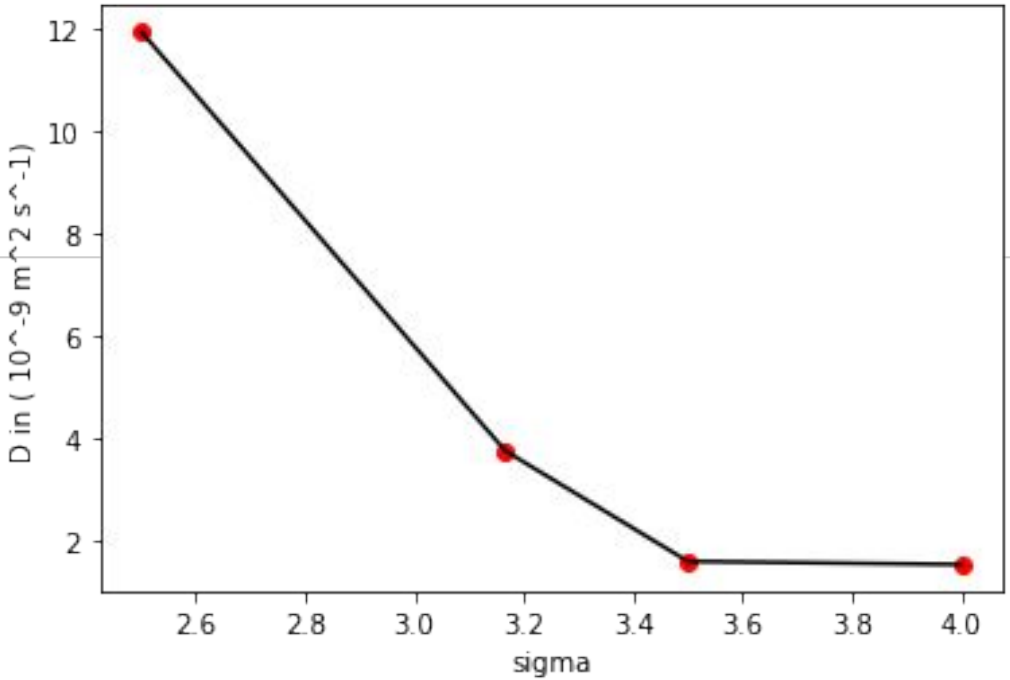
Diffusion Coefficient (D)

D = MSD/6t

From the above relation, the diffusion coefficient is calculated from the slope of MSD vs time graph,

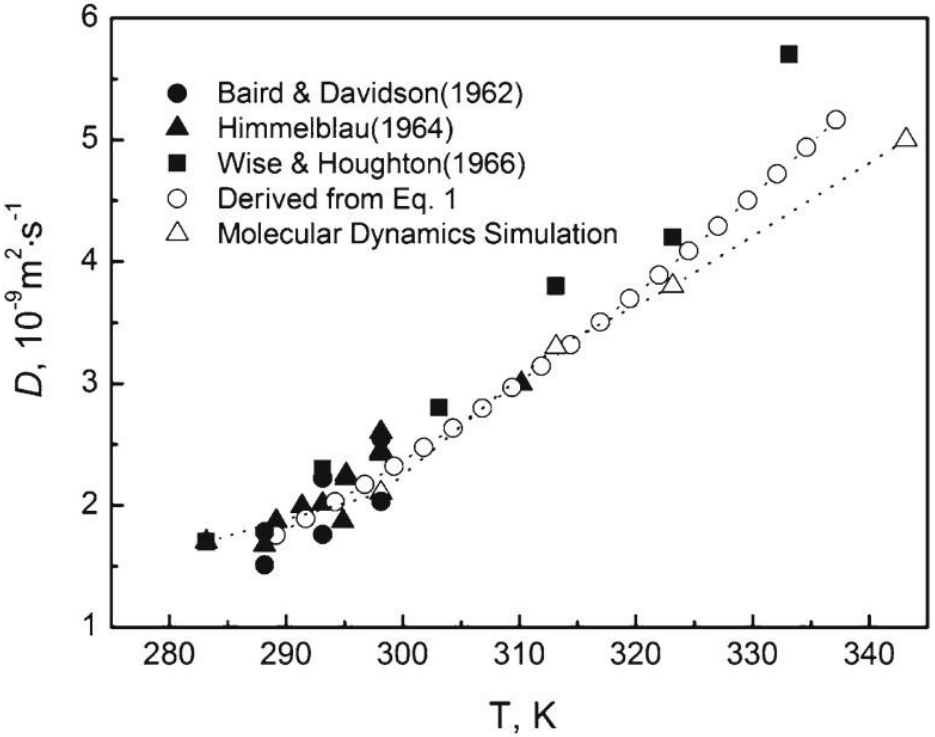
sigma	Diffusion Coefficient in (10^-9 m^2 s^-1)
2.5	11.93
3.166	3.74
3.5	1.58
4	1.52

Variation of Diffusion Coefficient over Sigma values



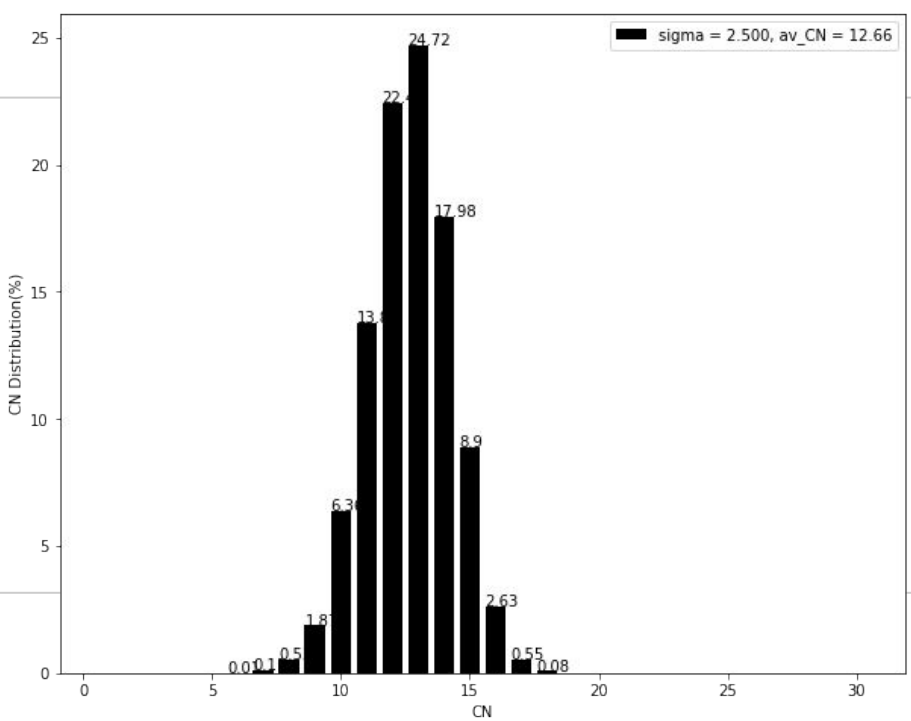
The Diffusion Coefficient values are observed to saturate with increasing sigma values

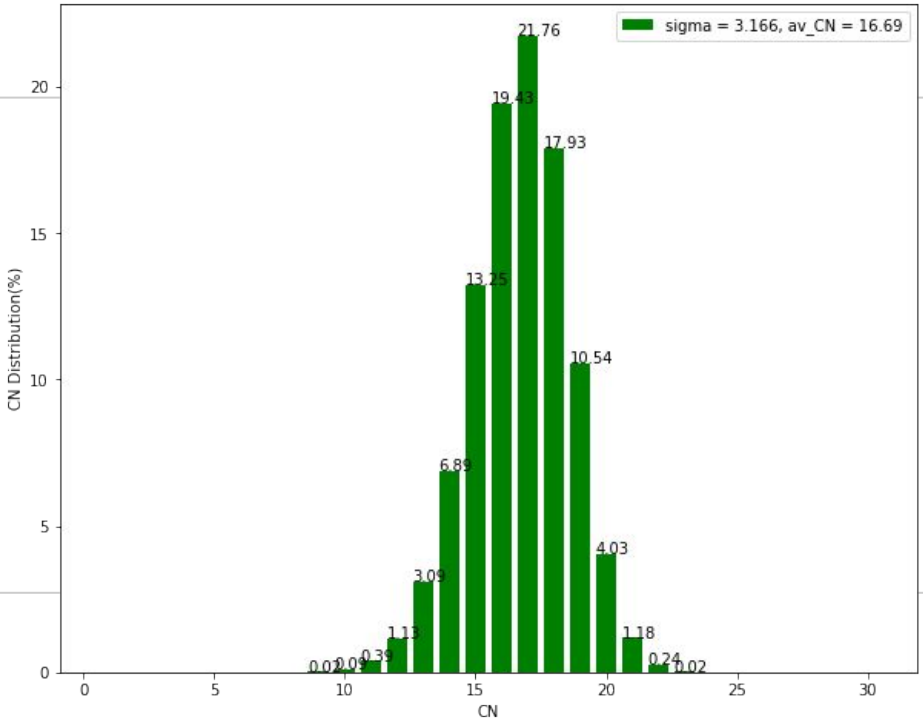
Diffusion Coefficient (D) comparison from Literature



Reference : A Molecular Dynamics Simulation of the Diffusivity of O2 in Supercritical Water

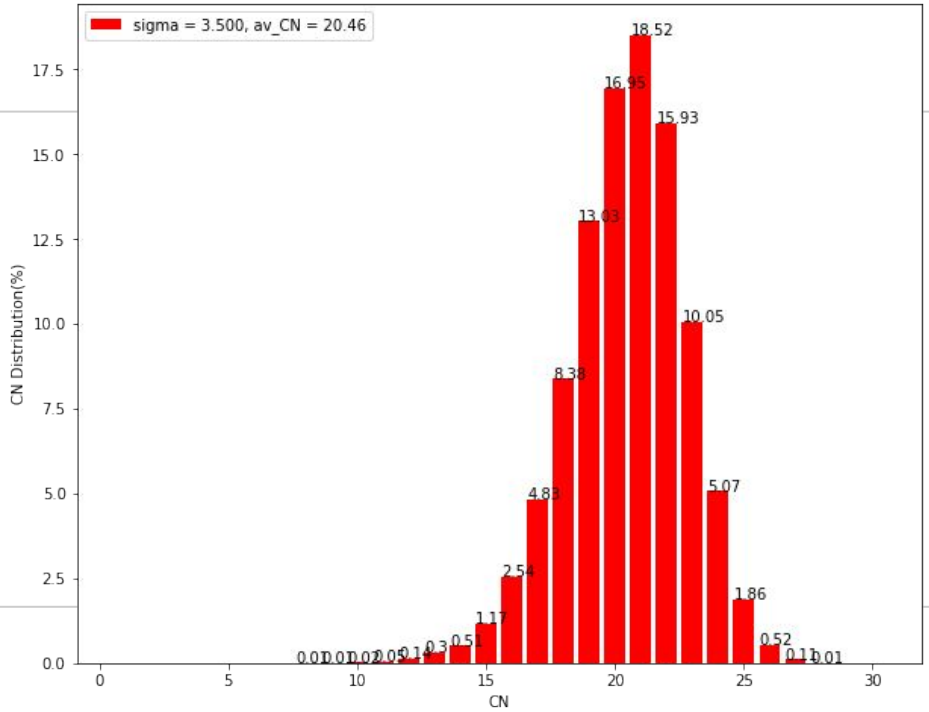
Coordination Number Density

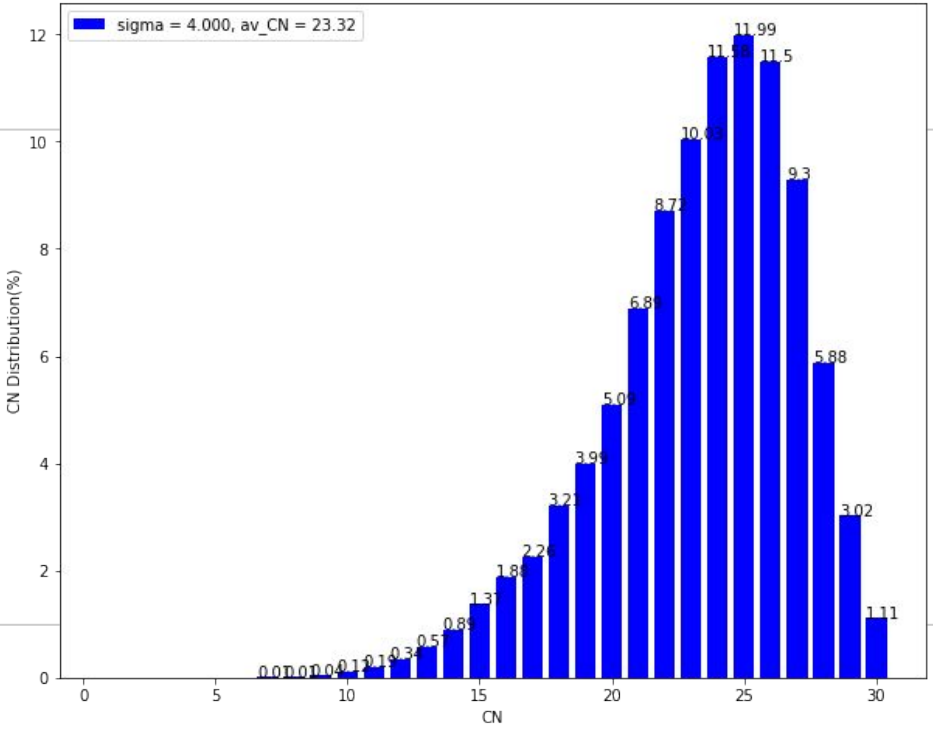




Larger sigma values have more spread out distribution

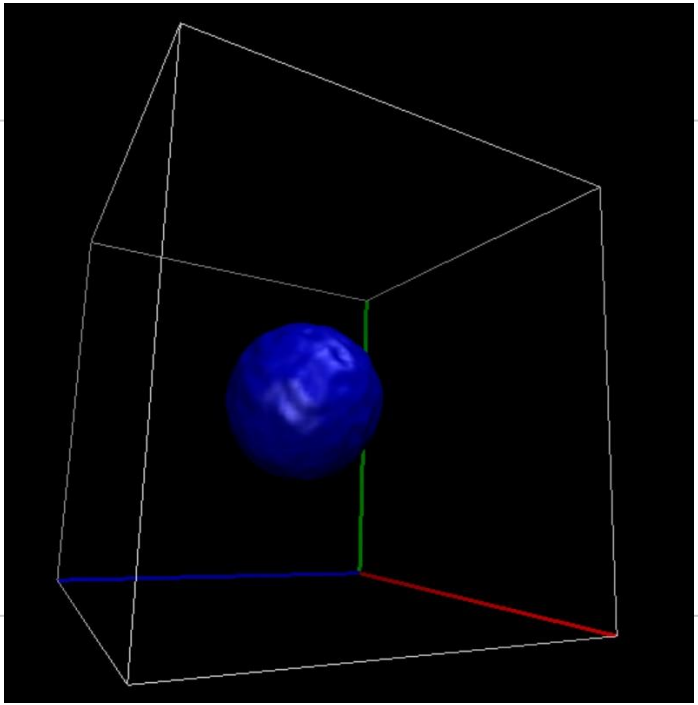
Coordination Number Density



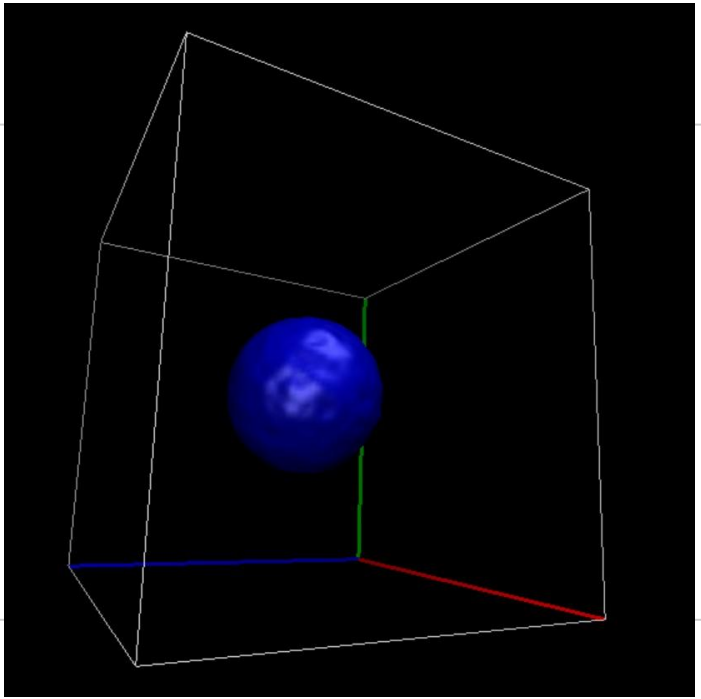


Average coordination number is increasing with increase in sigma values

Spatial Distribution Function



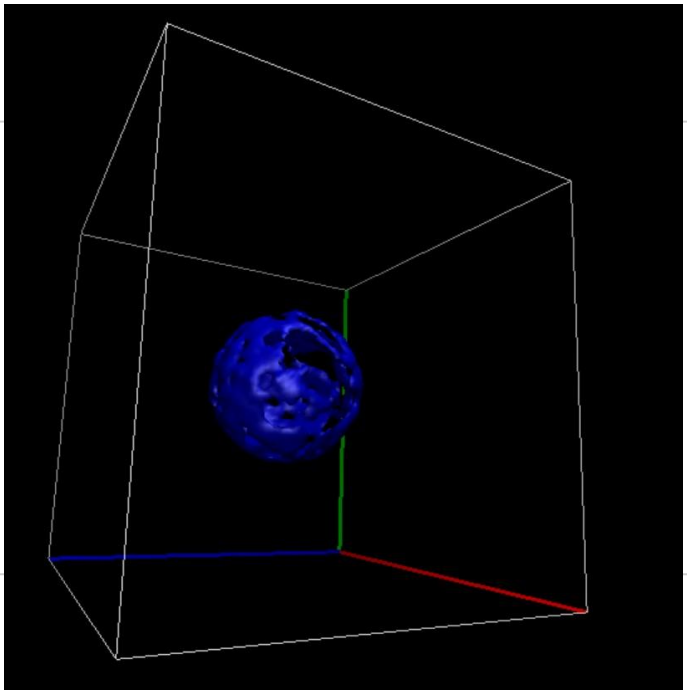
Sigma = 2.500



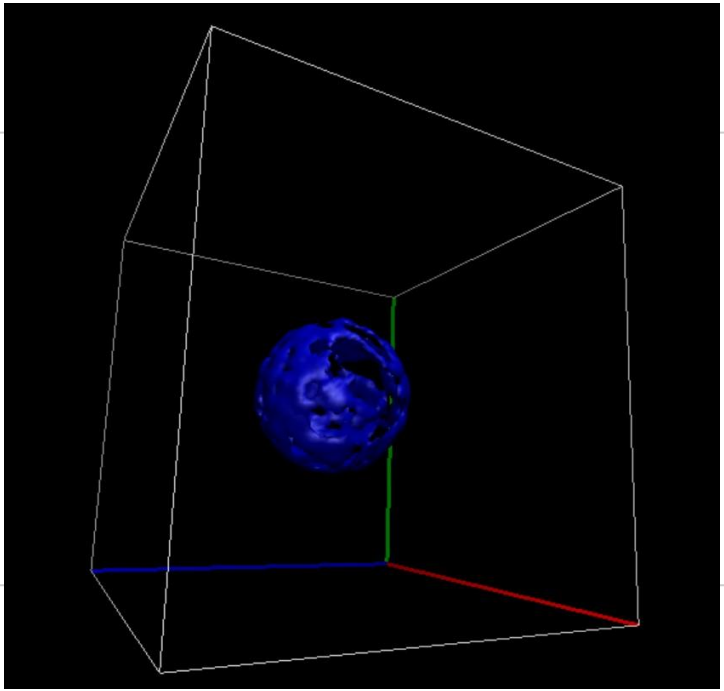
Sigma = 3.166

For Isovalue = 18

Spatial Distribution Function



Sigma = 3.500



Sigma = 4.000

For Isovalue = 18

Conclusion

- RDF plots with variation of sigma values is in agreement qualitatively with reference.
- Diffusion coefficient is exceptionally high for sigma = 2.500.
- MSD plots are fairly straight.
- Coordination number gets more largely spread out with increase in sigma values.
- Average Coordination Number also increase with increase in sigma values.
- Spatial Density Function has more well defined shells with decreasing sigma values.

Thanks!

Any questions ?