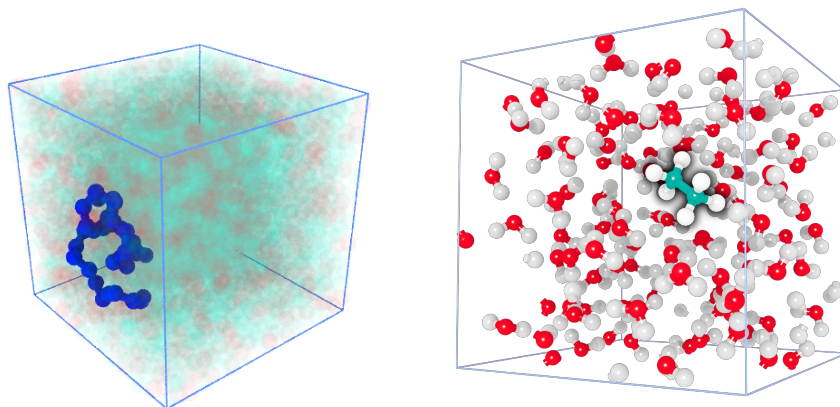


7th Tutorial on MD - Tying Up Loose Ends: Visualization, Mixing Rules and Atomistic MD Simulations

Today we will look at Lennard-Jones parameters again. We will learn how to handle the situation when some atom types have different potential depths and minima positions, and how they interact with the other particle types. Then, if some time is left, we will have a short look at how MD simulations can be performed with atomistic systems, i.e. in real units and using models that represent realistic atoms and molecules.



Visualizing Your Systems

Some basic advice before we start: If you want to get a feeling for your system it is a good idea to visualize it. I can recommend the program OVITO, which is quite user-friendly. You can download it at <https://www.ovito.org> or on the IPF website on the exercises/scripts page. Choose the Basic version that suits your operating system. Inside OVITO you can directly load LAMMPS Data files and look at them. You can also add so-called modifiers. This allows you, for example, to select parts of your system and to hide them or to load trajectories showing the movement of your molecules.

Mixing Rules

The Lorentz-Berthelot combination rules provide the parameters for the interaction energies between dissimilar atom types. This typically only concern the van-der-Waals part of their pair interaction energy, in our simulations represented by Lennard-Jones potentials.

- Lorentz rule (effective radii between two particles): $\sigma_{ij} = \frac{\sigma_{ii} + \sigma_{jj}}{2}$
- Berthelot rule (effective potential depth): $\epsilon_{ij} = \sqrt{\epsilon_{ii}\epsilon_{jj}}$
- Short cutoff (repulsive): $r_{cut,ij} = \sqrt[6]{2}\sigma_{ij}$
- Long cutoff (attractive): $r_{cut,ij} = 2.5\sigma_{ij}$

Co-Non-Solvency Effect

Investigate the influence of a binary solvent mixture on the spatial extension of a single polymer chain. What happens when a polymer chain is exposed to two good solvents (both are attractive to the chain), but their attractivity is different?

1.) The given starting configuration (`chain.data`) contains a polymer chain (*type 1*) and a monomeric solvent (*type 2*). Set up a range of new starting configurations, in which a fraction of the original solvent particles will be co-solvent (type 3), which will be more attractive. Vary the co-solvent concentration c from 0.0 to 1.0 in 4 to 5 steps.

2.) Assign the Lennard-Jones Parameters in the LAMMPS input file provided. Use the following parameters - first fill the remaining ones based on the Lorentz-Berthelot rules:

type i	type j	ϵ_{ij}	σ_{ij}	r_{cut}
1	1	1.0	1.0	repulsive
1	2	0.5	$\sigma_{1,2}$	attractive
1	3	1.0	$\sigma_{1,3}$	attractive
2	2	1.0	0.5	repulsive
2	3	$\epsilon_{2,3}$	$\sigma_{2,3}$	repulsive
3	3	1.0	0.5	repulsive

3.) Run the simulations for the different concentrations - first equilibrating, then production run. For the second part, perform a measurement of the radius of gyration. You can do it in LAMMPS or you write out the trajectory and measure R_g later.

4.) Plot the results of $R_g(c)$ as a function of the co-solvent concentration (between 0 and 1.0). Normalize the values of $R_g(c)$ by the value at $R_g(c = 0)$. What effect do you observe? Is this expected - why or why not? How can it be explained?

Atomistic Simulations

This part is meant to give you a basic idea how to simulate fully atomistic models of molecules. We will look at the LAMMPS Data file and the input scripts and what changes to simulate a simple system, here Ethane (DREIDING force field) solvated in water (SPC/E model).