2nd Tutorial on MD: Kremer-Grest Model and Working with Observables

Today we are taking a look at a simulated polymer melt in equilibrium and aim to investigate some basic properties. The melt consists of $M = 100$ polymer chains of equal degree of polymerization $N = 30$. We have a file *unwrapped.txt* containing 51 snapshots of the simulation, with each snapshot containing the coordinates of the monomers.The simulation has been performed with the MD simulation package `LAMMPS`, that is available for free and is used widely for molecular dynamics simulations. The chains here are represented in the so-called "Kremer-Grest model", which is one kind of "bead-spring model" of polymers.

More detail on the tasks and background information is provided in a jupyter notebook *MD2-Students.ipynb* (and *MD2-Full.ipynb* for the solutions).

Reading the file and extracting basic parameters

1.) Read in the file *unwrapped.txt* the trajectory of the polymer melt. First, take a look at the format of the file - what information is stored in what lines? After reading in the fold, the trajectory of the melt should be stored in a numpy array (Hint: Read it line by line).

2.) Extract some basic parameters of the system from the file, e.g. box dimensions, box volume, number of monomers, number density of monomers, number of chains, monomers per chain, number of snapshots, etc.

Bonds in the Kremer-Grest model: The FENE potential

$$U_{\mathrm{FENE}}(r) = -\frac{1}{2}K \cdot r_0 \cdot \ln\left(1 - \frac{r}{r_0}\right), \quad r < r_0$$

3.) Plot the FENE potential and the LJ potential as well as their sum. Find the minimum of the combination of $U_{\mathrm{LJ}}(r) + U_{\mathrm{FENE}}(r)$ and print it to the screen.

4.) Assuming we are in equilibrium, calculate the average bond length of the simulated melt.

End-to-end distance $\vec{R}$

5. a) Calculate the end-to-end distance vector $\vec{R}$ of the chains (and its average $\langle vecR \rangle$) as well as its average length R. What values are to be expected?

5. b) Use this calculation to also find and plot the autocorrelation function $\langle \vec{R(0)} \cdot \vec{R(t)} \rangle$ of the end-to-end vector. Fit it with a decaying exponential function of the form $\exp(-t/\tau_1)$ to find the largest relaxation time (also "Rouse time") τ_1 of the system

Radius of gyration R_g

$$R_g^2 = \frac{1}{N}\sum_{i=1}^{N}\left(\vec{R}_i - \vec{R_{cm}}\right)^2,$$

$$\vec{R_{cm}} = \frac{1}{N} \sum_{j=1}^{N} \vec{R_j}.$$

6.) Calculate the average radius of gyration $\langle R_g \rangle$ of the polymer chains.

7.) Compare the (squared) radius of gyration and the (squared) end to end distance. What is the ratio between them ? Can you verify the theoretically expected value? (Hint: Best to calculate $\langle R^2 \rangle / \langle R_g^2 \rangle$)