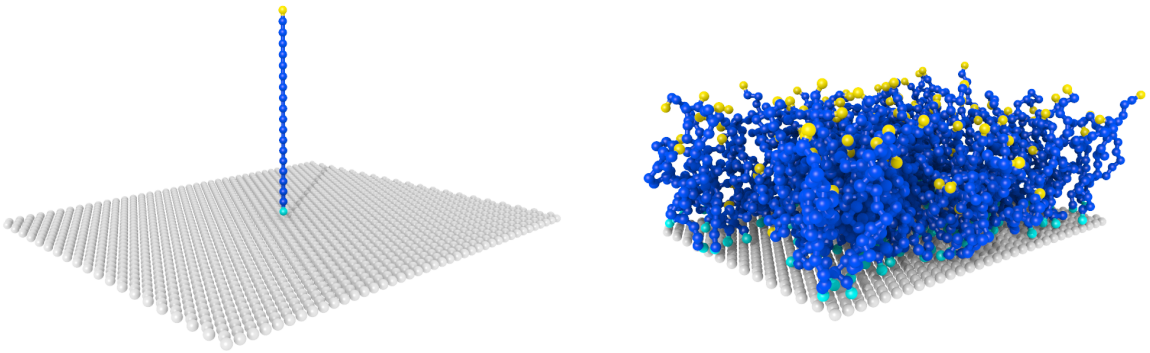
4th Tutorial on MD - End-tethered polymer chains

Today we continue using LAMMPS and we will learn some more of its functions: how to select groups of atoms, how to apply certain manipulations to them etc. As an example system, we consider a polymer chain that is attached to a wall of atoms by one end. We will get to know. Later we will have a look at polymer brushes.



Single Chain on a moving wall

You receive commented LAMMPS scripts `in.langevin` (in the folder `langevin`) and `in.dpd` (in the folder `dpd`). Using these, we will simulate an end-thethered polymer chain on a wall moving at constant velocity - this setup is saved to the file `start.data` in both folders.

1.) Have a look at start.data and identify the different parts of the system and their particle type.

2.) Open `in.langevin` and identify what settings are already made. To complete it make the following edits:

- Define seperate "groups" for the wall, the chain and the two different chain ends.
- The chain should always remain attached to the wall of atoms (How is this realized?).
- The wall should move at a constant velocity $v = 0.5$ along the x-direction.

3.) Next, run the simulation. Make sure that two output files will be created:

- `z.txt` contains the z-position of the chain end as a function of time.
- `rg.txt` contains the radius of gyration R_g of the chain as a function of time.

4.) Do tasks 2 and 3 for `dpd/in.dpd`. After this simulations has also finished, plot the results of both - one figure for `z.txt` and a second one for `rg.txt`. What do you observe? What happens to the two pulled chains in the different simulations? Is it realistic - when and why?

Polymer brush

5.) Consider how the system would have to be changed to now simulate a polymer brush. What conditions need to be met? What does density brush profile of a brush look like (histogram of partcile positions along z)? How are the ends of the chain distributed within the brush?

6.) Go into the folder `brush` and open the file `brush_N20.data`. What has changed and what is the same when compared to the previous file `start.data`?

7.) Use the provided script `in.brush` to run the simulation. Then plot the two files `rho.data` (density profile of the chain along z) and `ends.data` (chainnd profile along in z). Compare to your predictions. How do the histograms need to be normalized to get density units (particles per volume)? What is the height of the brush?

8.) Identify from the given information (within the files and written out by LAMMPS) the grafting density of the brush, $\sigma = n_{chains}/A$ (chains per area).