

# 2nd Course Assessment - Molecular Dynamics

For the second course assessment you receive this exercise sheet (*two pages!*) plus LAMMPS scripts and data files. You need the simulation software LAMMPS to handle the simulations. In total, you have **90 min** to solve the tasks. You can use all materials that were provided during the lectures and exercises. In a short protocol (German or English) ***briefly*** document:

- the answers to the (direct) questions,
- your results, i.e. any calculations, numbers, plots, descriptions or interpretations.

## 1. Lennard-Jones Particles in a Box

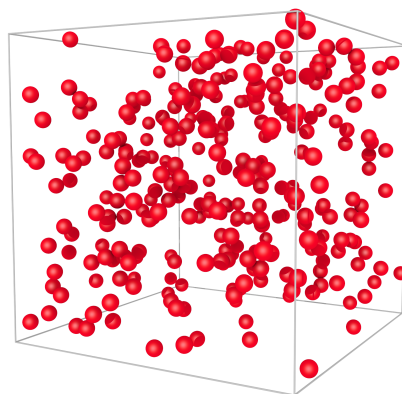
The folder LJ contains a prepared LAMMPS script `in.LJ`. It simulates a 3-dimensional NVT system of Lennard-Jones particles including attractive interactions. After an equilibration period the script regularly writes out a LAMMPS dump file `wrapped.txt` containing the particle coordinates. You can modify the script to set the temperature  $T$ .

1.1.) Create three folders, to perform three simulations. Copy the script in there and perform the simulations at temperatures  $T = 0.1$ ,  $T = 0.5$ , and  $T = 1.5$ . Extract the number density  $\rho = N_{\text{atoms}}/V$  of the system from the information LAMMPS provides.

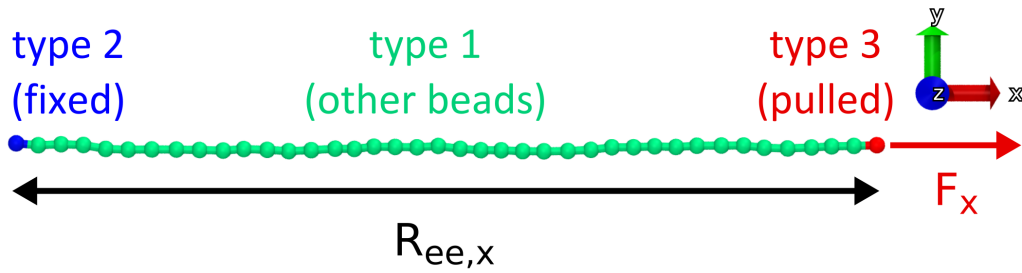
1.2.) Calculate the radial distribution function  $g(r)$  for each of the three simulated systems. For the given system, what is the maximum distance  $r$  that can be resolved in the radial distribution function? Why is it not meaningful to consider larger distances?

1.3.) Plot  $g(r)$  of each simulated system in **separate figures**. Use a suitable bin size, normalization, etc.

1.4.) For each system, describe the curve  $g(r)$  and interpret the state of the system (aggregation state, how are the particles distributed).



## 2. Pulled Ideal Chain



The folder `chain` contains a prepared LAMMPS script `in.pull` and a data file `chain.data`. Using these files you can simulate an ideal chain (excluded volume *off*) of  $N = 40$  monomers (*type 1*) with one spatially fixed end monomer (*type 2*). The other end monomer (*type 3*) can freely move and will be pulled by a force  $F_x$  in the  $x$ -direction. Over the course of the simulation the force increases in increments of  $\Delta F_x = 10$  (LJ units) between  $F_x = 0$  and 200. For each given value of  $F_x$  the chain extension along the  $x$ -direction  $R_{ee,x}$  is measured. The task is to investigate how the bonding potential influences the chain extension behavior. We consider two cases: bonding monomers by (a) harmonic springs or (b) the FENE potential (Finite Extensible Nonlinear Elastic).

Create two folders, `harmonic` and `fene`, and copy the LAMMPS files into them. In each folder, activate the suitable bonding potential (harmonic or FENE) using the given parameters in the script. You can activate a bonding potential by uncommenting the according section in the script.

2.1.) Run the two simulations. Each simulation will create a file `force_vs_x.txt` that stores  $R_{ee,x}$  and  $F_x$ . Plot these results, i.e. **plot both** resulting force-extension curves ( $F_x$  as a function of  $R_{ee,x}$ ) **into one figure**.

2.2.) Describe and compare the two force-extension curves. Interpret how the type of bonding potential (harmonic, FENE) results in the particular shape of the curve.

2.3.) Consider again the force extension curve of only the **harmonic** bonding potential. Suppose you are given just the plot  $F_x$  vs.  $R_{ee,x}$ . From this curve alone, how could you extract the parameters of the bonding potential connecting a pair of neighboring monomers in the chain? Show an example calculation for the given chain with  $N = 40$ . Reminder: in LAMMPS harmonic bonds are given by  $U_{\text{harmonic}} = K(r - r_0)^2$ .