1st Tutorial on Molecular Dynamics: A Simple MD Code

You will receive a jupyter notebook containing an incomplete program. **Complete the code and turn it into a simple but functional coarse-grained molecular dynamics (MD) code**, i.e. particles should move physically correct and some thermodynamic output should be printed to the screen. The incomplete program is already structured.

The system we want to simulate is a Lennard-Jones (LJ) fluid in the NVE ensemble. Spherical particles are interacting via the LJ potential and move because we time-integrate Newton's equations of motion by using the Velocity-Verlet algorithm. NVE means we conserve particle number N, simulation box volume V and total energy E.

0.) Open the jupyter notebook file `MD1-Studenty.ipynb`, where you will find more detailed instructions. Familiarize yourself with the structure of the program. Which program parts are necessary for a minimal functioning MD simulation? Which parts need to be filled in?

Basic Simulation Parameters and Lennard-Jones Potential

1.) Define the basic parameters of the simulation, e.g. number of particles, size of the box, timestep, interaction potential (LJ potential), etc.

2.) Play around with the parameters of the LJ potential (ε, σ and r_{cut}) and plot a few different cases. Where is the minimum of the LJ Potential? Which cutoff r_{cut} has to be chosen to exclude any attractive forces?

Creating Particles and Their Initial Setup

3.) Define a class containing the necessary information of all particles. Initialize them so that all particles are inside the box and they do not overlap (e.g. on a simple grid). Assign randomized starting velocities to the atoms as well.

Verlet Integration and Thermodynamic Observables

4.) Write the functions which calculate positions, velocities, accelerations, and forces at each new timestep. We will later call them in the main loop to implement the Velocity-Verlet algorithm.

5.) Write a function *"compute"*, that calculates thermodynamic observables from atomistic information in regular intervals and prints them to the screen. At first, calculate potential energy, kinetic energy, total energy, temperature, and average particle velocity.

6.) Implement the Velocity-Verlet algorithm in the main loop and print thermodynamic information to the screen regularly, e.g. every 100 steps.

Optional Tasks

I.) Calculate the pressure of the system and print it to the screen with the other observables.

II.) Save the particle trajectory in regular steps to a file in the xyz-format. This file format can be opened with programs like VMD to watch the particles move like in a film.

III.) Calculate the radial density function *g(r)* of the system.