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Übungsblatt 2

The Lennard-Jones Fluid

1 Different cutoff schemes

We consider a system of 512 Lennard-Jones particles in a cubic box with 3.2 nm box length. We assign zero initial velocities to all particles. The simulation is started from a simple cubic lattice configuration. The Lennard Jones parameters should resemble argon atoms: $\sigma = 0.3401$ nm and $\varepsilon = 0.9786$ kJ/mol.

a) How does the simulation system evolve in time? What is the final temperature?

b) The system is simulated with

- a potential cutoff of 0.9 nm
- a potential cutoff of 1.1 nm
- a shifted potential with cutoff 0.9 nm
- a switched potential with cutoff 0.9 nm

How does the energy evolve with time?

2 Constant temperature MD

a) We perform simulations of the same system as above at a constant temperature of $T = 188$ K with the weak-coupling algorithm with relaxation times of 0.01, 0.1, and 1 ps. Plot the energy and temperature as a function of time. What can you say about the stability of the algorithm? Calculate the relative variance of the temperature

$$\frac{\langle T^2 \rangle - \langle T \rangle^2}{\langle T \rangle^2}.$$

Plot the distributions of the particle veolcities.

b) Restart the simulation with the final coordinates and velocities, now using a temperature of 300 K. Plot the energy and temperature as a function of time.

c) Perform the same steps for a Nose-Hoover thermostat.

3 System size dependence

Perform a simulation of the same LJ fluid with systems of 512, 1024, 2048, and 4196 particles. Plot the relative temperature fluctuations as a function of N. What scaling do you observe?

4 Constant pressure MD

a) We perform simulations of the same system as above but now in the NPT ensemble at 188 K and 400 bar. We use an isotropic weak-coupling algorithm with pressure relaxation times of 0.01, 0.1, and 1 ps. Plot the energy, pressure, and box volume as a function of time. What can you say about the stability of the algorithm. Calculate the relative variance of the pressure

$$\frac{\langle P^2 \rangle - \langle P \rangle^2}{\langle P \rangle^2}.$$

What consequence follows for the stability of the method?

b) Perform the same steps with a Nose-Hoover thermostat and an isotropic Parrinello-Rahman barostat.

c) Perform the same steps with a semiisotropic weak-coupling barostat.

5 Supercritical isotherm

Calculate the reduced density ρ^* as a function of the reduced pressure p^* of the Lennard-Jones model of argon for the reduced temperature $T^* = 1.6$. Plot p^*as a function of $1/\rho^*$.