Molecular Dynamics Simulations 2025 / Exercise 1

To be handed in latest before the exercise session on Thu Dec 7. Guidance will be given at exercise session on Thu Nov 30 A127/Chemicum 10:15. Solutions will be revealed at the exercise session Thu Dec 7 A127/Chemicum 10:15.

Return the exercise solutions using Moodle. See instructions from the first lecture on how to make the return.

In this exercise, the objective is to get one to familiarise with the different basic concepts involved in molecular dynamics and obtain a minimum working example with a popular MD code, such as LAMMPS and a visualisation tool such as OVITO.

1. Using lammps, create a diamond cell of Silicon 2x2x2 unit cells. To describe the interatomic interaction between particles in the system use the Stillinger-Weber potential, provided with the exercise instructions. Minimise it's positions, generate velocities using a gaussian distribution at 300 K, seed 123456 and preserving the linear and rotational momentum. Relax the system at 300 K in NPT for 30 ps and constant tau. Then, relax it for another 30 ps using the NVT thermostat [1]. Save thermo output every 100 steps[2] . Plot

- The energy, pressure, and temperature as a function of time
- The pair correlation function as a function of time. You can plot it every 5 ps.

2. Using the previous script convert all the previous parameters to placeholder variables, which can be parsed from the command line, and test the following:

- Check timesteps: 0.0001, 0.0005, 0.001, 0.003, 0.01 ps. Plot energy vs timestep for each. Comment on what you observe.
- Monitor the temperature as a function of time for different temperature relaxation constant. Do you see any difference?
- Monitor pressure as a function of time for different simulation cell sizes (N=1, N=2, N=4, N=8). What conclusions do you draw?

Based on the previous plots, what are the optimal parameters of your simulation? Reason your choice.

3. For this part of the exercise use dt=1e-3 ps; τ_T = 0.1; τ_P = 1.0 and N = 6. Equilibrate your cell for a temperature range going from 200 K to 400 K, in steps of 10 K. Extract the length of your simulation cell (not the volume which scales as a cubic function) after equilibration. Plot the difference of the cell size and the size at 300 K against temperature (the curve should cross the 0 at 300 K). From your results extract the thermal expansion coefficient α at room temperature (300 K) by fitting the function $a(T) = a_0(1+\alpha(T-T_0))$

[1] to stop the simulation at the right time you might want to use the "fix halt"

[2] When recording thermodynamic information for later plot, you may use the following line to add a unique word at the biggining of each relevant line, so they are easier to parse: thermo_modify line one flush yes format 1 "ec %8lu"