Lab 4

Classical Molecular Dynamics of Silver

May 2018

1 Problem 1 - Testing simulation parameters [35 points]

This first problem is about the convergence of the simulation parameters in order to be able to perform a simulation within the required precision. You should consult the Handout for detailed instructions.

A) Find a good timestep for the highest simulated temperature, by looking at which timestep the constant of motion is still conserved. For conserved runs, give the amplitude of fluctuations of the conserved quantity as a function of timestep. [10 points]
OPTIONAL: How do the fluctuations in the conserved quantity (the total energy) scale with the timestep? Discuss your result, referring to what you learned about the error in the integration with a Verlet algorithm.

B) Converge the system supercell size to get the fluctuations in the temperature below a threshold. How do the fluctuations decrease with increased system size? [10 points]

C) Estimate the ideal production length from the velocity auto-correlation function $VAF(t)$ at the lowest temperature ($1000K$). Explain in one sentence why one should make this

estimate at the lowest temperature. Derive how the value of $VAF(t = 0)$ is related to $\langle E_{kin} \rangle$, and check this for one of your trajectories. [15 points]

2 Problem 2 - Melting of bulk silver [45 points]

In this problem, MD simulations within a constant temperature (NVT) ensemble will be used to obtain the melting of bulk silver. For this task you will be required to consider a significant number of different temperatures, ranging from values below the experimental melting point to temperatures significantly above it. See the Handout for more details.

A) Create a plot of the potential energy per atom as a function of temperature, otherwise known as the caloric curve. When your material undergoes a phase transition from liquid to solid, you should see a discontinuity in the curve. Provide an estimate of the melting temperature based upon these results. [10 points]

B) Plot the radia distribution functions (RDFs) for different temperatures and estimate the melting temperature based on the comparison. Estimate the coordination number for temperatures below and temperatures above the melting point by integrating the RDF. [10 points]

C) Calculate the diffusion coefficients from the mean square displacement (MSD). Determine the melting temperature by identifying the transition to net-diffusive behavior. For all simulations in the liquid phase, generate a plot of $log(\mathrm{D})$ as a function of $1/T$. What is the slope of this function and what is its physical interpretation? [15 points]

D) Compute (and plot) the fixed-volume specific heat as a function of temperature, across the melting point, and estimate again the melting temperature with this methodology. [10 points]

NOTE: Make sure to document all relevant simulation parameters. Discuss your results, and make sure you explain how you arrived at your conclusions.

3 Problem 3 - Scalability of MD systems (20 points)

Consider a bulk material simulation using periodic boundary conditions and large supercells.

A) For fcc materials, how many atoms are contained in a supercell consisting of $N \times N \times N$ unit cells? How many force calculations are required for each timestep if all atoms are considered? How many force calculations are required if a potential cutoff is implemented? How many times must you calculate the distance between atoms? Provide another possible strategy to optimize MD simulations. [10 points]

B) Rank the following force calculations in terms of the CPU time required: Hartree-Fock methods, Lennard-Jones pair potentials, EAM pair functional potentials, and density-functional theory. Explain your choices. [10 points]