NB: The graded, first version of the report must be returned if you hand in a second time!

H1a: Classical scattering by a central potential

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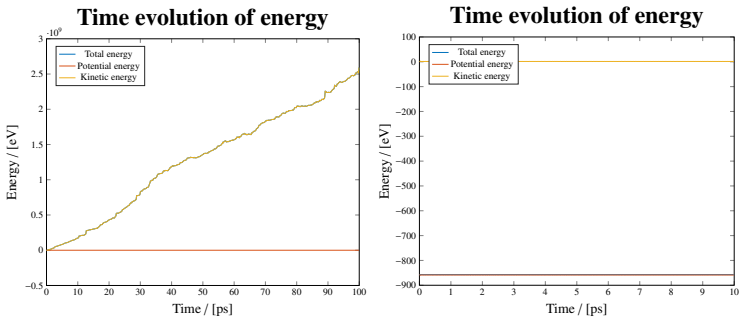
Task №	Points	Avail. points
Σ		

Introduction

Molecular dynamics is a simulation of the movement of atoms and molecules. What is of interest in such a simulations is e.g. the trajectories of the atoms given specific surrounding parameters such as temperature, pressure, crystal formation etc. For this homeproblem we study the dynamics of aluminium atoms in a FCC crystal lattice.

Problem 1



(a) $\Delta t = 0.1$ ASU (b) $\Delta t = 0.01$ ASU

Figure 1: For the different energy simulations, the same number of timesteps was used but the lengths of the different timesteps makes them evolve over different times. As can be seen in 1a, the energy explodes due to insufficient resolution of the time, something which is not present in 1b.

As we can see in figure 1 the required timestep is between $\Delta t = 0.1 \sim 0.01$ ASU, so for the rest of the assignment a timestep of $\Delta t = 0.01$ ASU will be used.

Problem 3

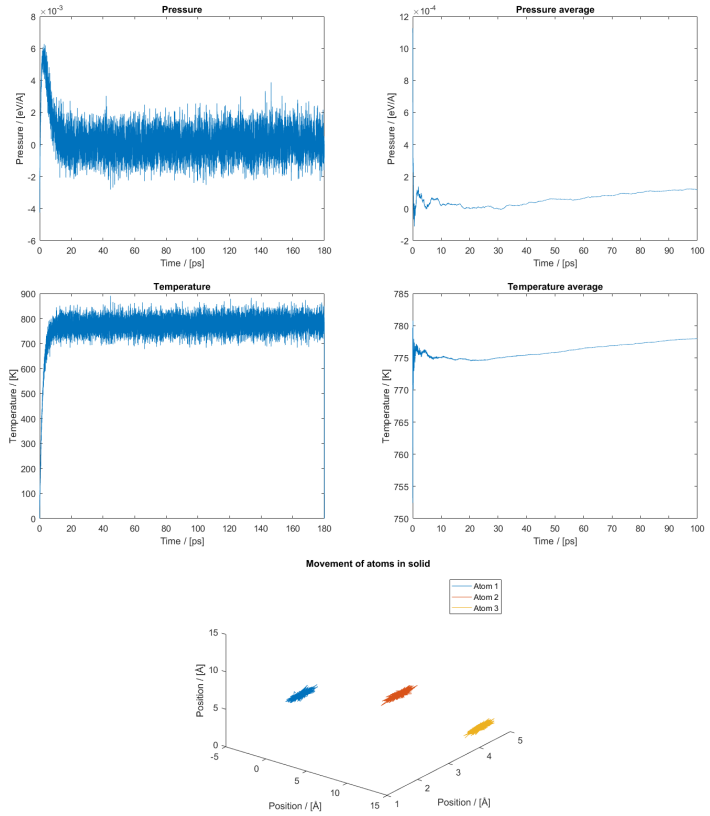


Figure 2: After the equilibrium, both the pressure and the temperature needs some time to stabilize after rescaling the velocities, but remains stable for longer time. The equalisation temperature was set to 500 C°.

In order to set the system to a certain temperature, a technique involving scaling all the velocities during a equilibrating state. Since the temperature depends on the kinetic energies which in turn depends on the velocities, the temperature can thusly be changed by changing velocities. In figure 3 we can see the temperature after setting the temperature to 500 C°. There are some fluctuations in the beginning due to the rescaling of the velocities.

Problem 4

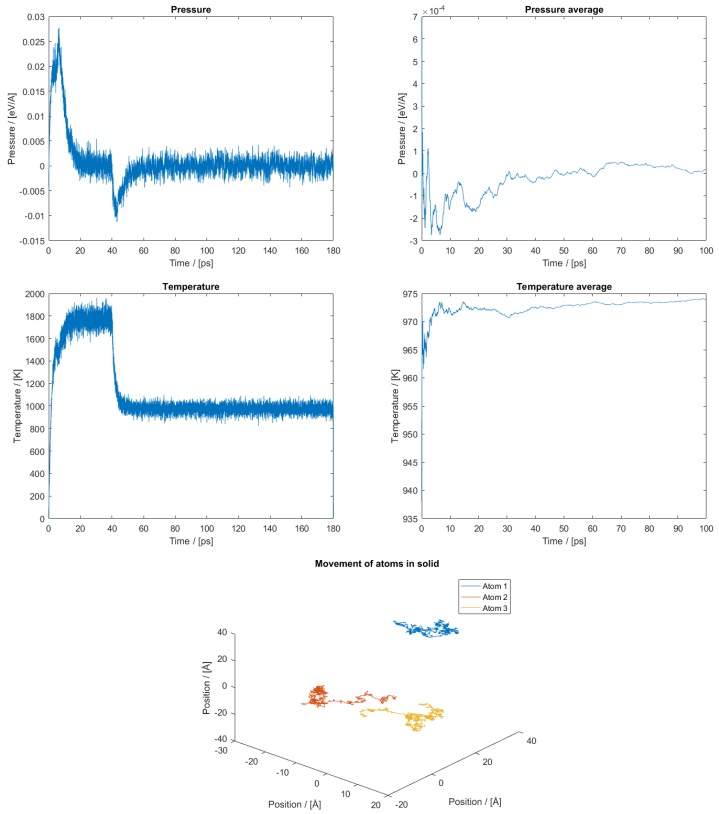


Figure 3: After the equilibrium, both the pressure and the temperature needs some time to stabilize after rescaling the velocities, but remains stable for longer time. The equalisation temperature was first set to 1000 C° for the smelting and then the temperature was reduced to 700 C°.

Problem 5

$1\ \frac{\mathrm{j}}{\mathrm{molK}} = 1.0366e-05\ \frac{\mathrm{eV}}{\mathrm{K}}$
$C_v\ [AL] : 24.20\ \frac{\mathrm{j}}{\mathrm{molK}} = 1.0366e-05\ \frac{\mathrm{eV}}{\mathrm{K}}$
From our MD simulations we obtained the following values for C_V when using the potential and kinetic energy fluctuations respectively.

Table 1: Heat capacity obtained by measuring energy fluctuations.

Temperature	**500° C**	**700° C**
$C_V/(\mathrm{eV/kg\,K})$ (kinetic)	$5.819521 \cdot 10^{-2}$	$5.056438 \cdot 10^{-2}$
$C_V/(\mathrm{eV/kg\,K})$ (potential)	$5.836188 \cdot 10^{-2}$	$5.056541 \cdot 10^{-2}$

Problem 6

When instead using the relation

$$C_V = \left(\frac{\partial E}{\partial T}\right)_{N,V} \tag{1}$$

to compute the heat capacity, and approximate it with a difference quota, we obtain the results found in the table below.

If we compare these results to those from the previous problem we see that they are slightly larger and the result for 700 degrees deviates by a larger margin. It's possible

Table 2: Heat capacity obtained by approximating the partial energy derivative with respect to the temperature.

Temperature	**500° C**	**700° C**
$C_V/(\text{eV/kg K})$	$6.436 \cdot 10^{-2}$	$8.131 \cdot 10^{-2}$

that a longer equilibration time would yield a more stable temperature than was obtained now and therefore a more accurate heat capacity. A longer measuring time would also increase the accuracy of the result, as well as doing more simulation and averaging the different results. A ΔT of 5° C was used here, but further experiementing with this parameter could yield a better result as well.

Problem 7

The radial distribution function obtained can be found in figure 4. Using Matlab we find that the first peak is at the distance 2.8 Å, which corresponds to the closest distance between two aluminium atoms (shortest distance in a fcc structure with the unit cell length of 4.046 Å). This is expected. The other peaks

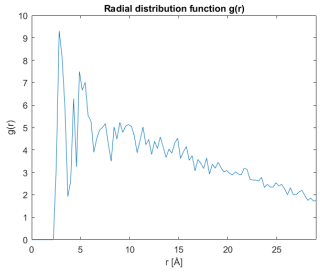


Figure 4: The radial function is computed by taking the histogram over all the internal distances between the atoms then divided by the random distribution of the same density.

Problem 8

Below (Fig. 5) are two approximations of the static structure function. The leftmost figure is obtained by integrating the result from Problem 7 and the rightmost one is obtained via simulation.

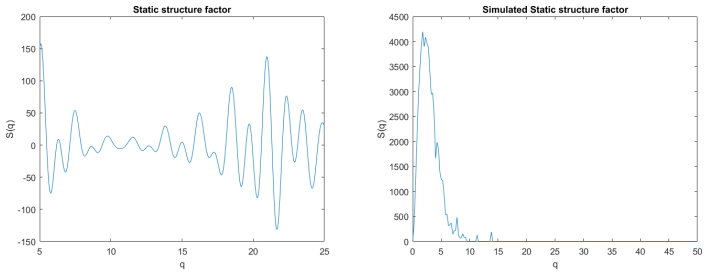


Figure 5: The static structure function computed both from the radial distribution function in figure 4 in the left and using bins in Fourier space to the right.