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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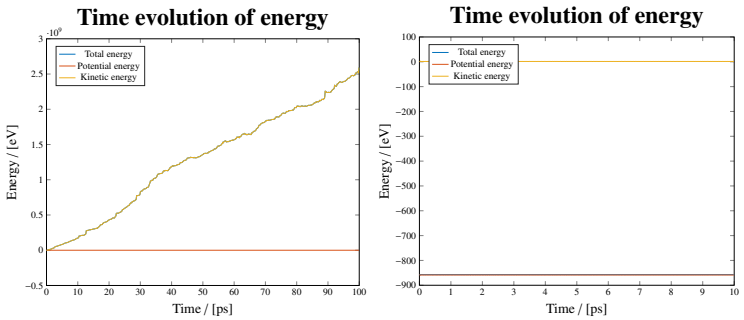
Task №	Points	Avail. points
Σ		

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

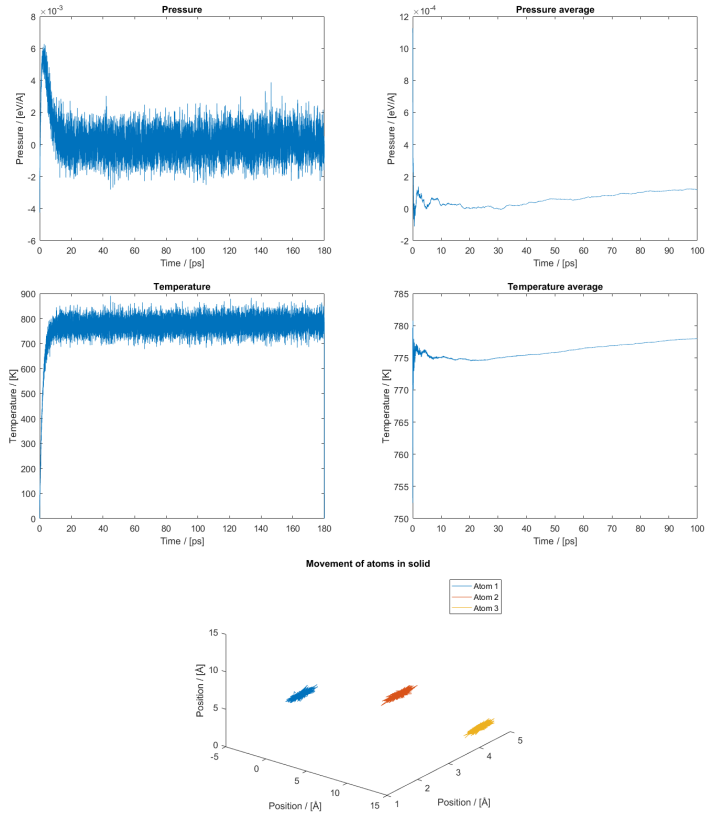


Figure 2: After the equilibrium, both the pressure and the temperature needs some time to stabilize after rescaling the velocities, but remains stable for longer time. The equalisation temperature was set to 500 C°.

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

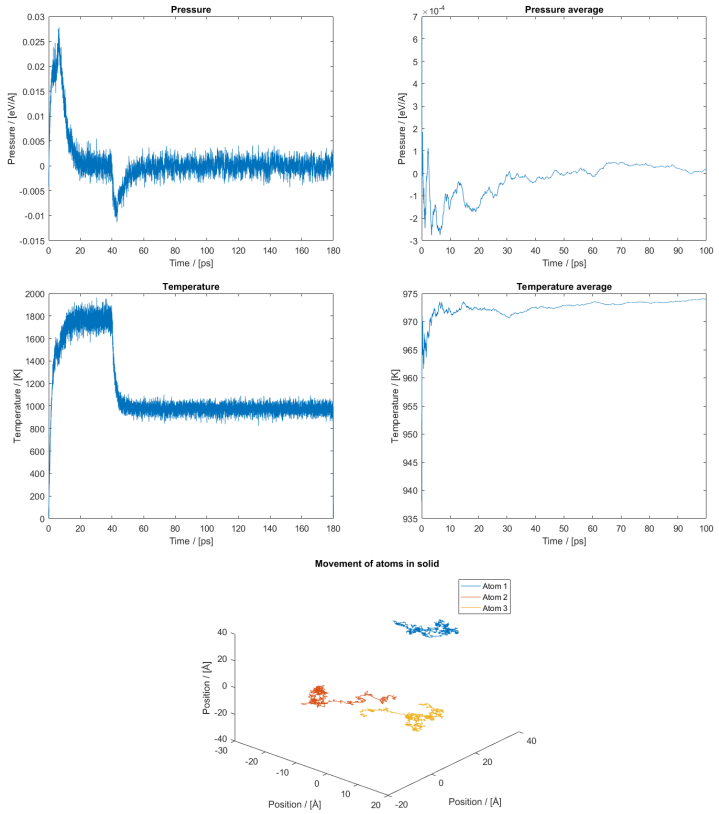


Figure 3: After the equilibrium, both the pressure and the temperature needs some time to stabilize after rescaling the velocities, but remains stable for longer time. The equalisation temperature was first set to 1000 C° for the smelting and then the temperature was reduced to 700 C°.

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

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 7

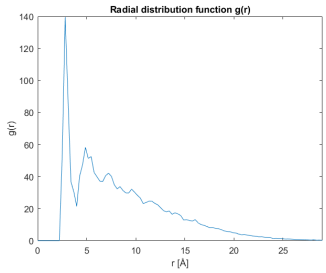


Figure 4: The radial function is computed by taking the histogram over all the internal distances between the atoms then divided by the random distribution of the same density.

Problem 8

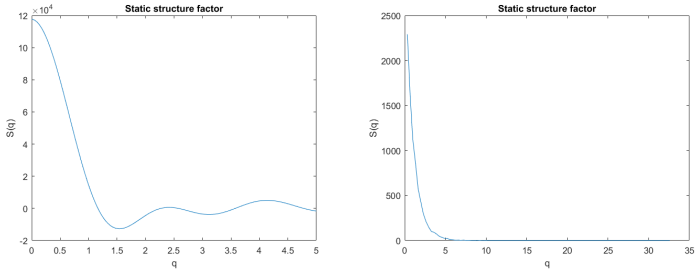


Figure 5: The static structure function computed both from the radial distribution function in figure **??** in the left and using bins in Fourier space to the right.