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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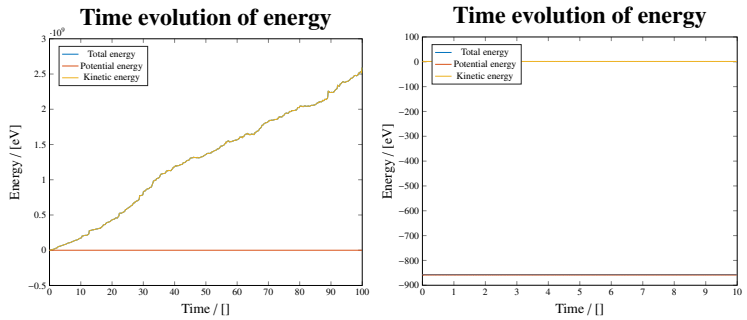
Task №	Points	Avail. points
Σ		

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

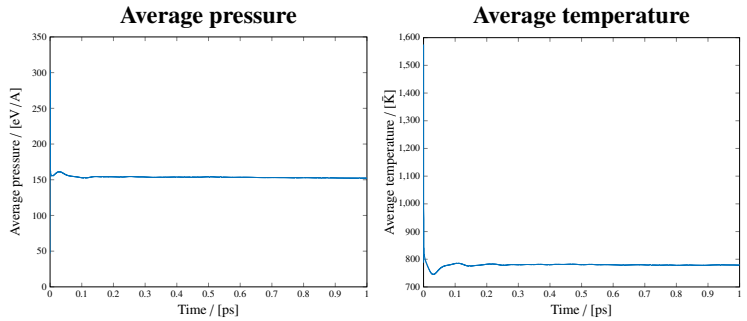


Figure 2: After the equilibrium, both the pressure and the temperature needs some time to stabilize after rescaling the velocities, but remains stable for longer time. The equalisation temperature was set to 500 C°.

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

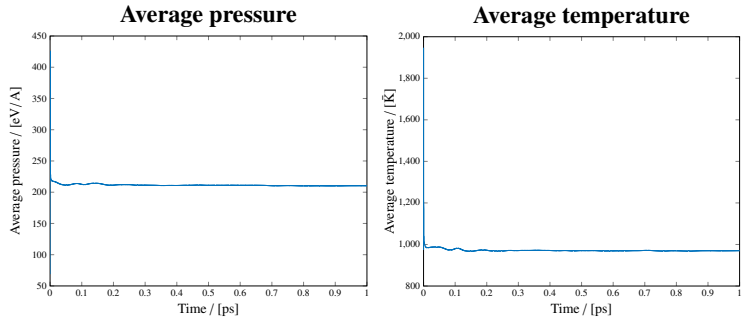


Figure 3: After the equilibrium, both the pressure and the temperature needs some time to stabilize after rescaling the velocities, but remains stable for longer time. The equalisation temperature was first set to 1000 C° for the smelting and then the temperature was reduced to 700 C°.

Problem 5

$1\ \frac{\mathrm{j}}{\mathrm{molK}} = 1.0366e-05\ \frac{\mathrm{eV}}{\mathrm{K}}$

$C_v\ [AL] : 24.20\ \frac{\mathrm{j}}{\mathrm{molK}} = 1.0366e-05\ \frac{\mathrm{eV}}{\mathrm{K}}$

As a starting point we first look at scattering from a hard-sphere potential. We also consider the Lennard–Jones potential, which is depicted in Figure 4. (*Always refer to Figures in the text.*)

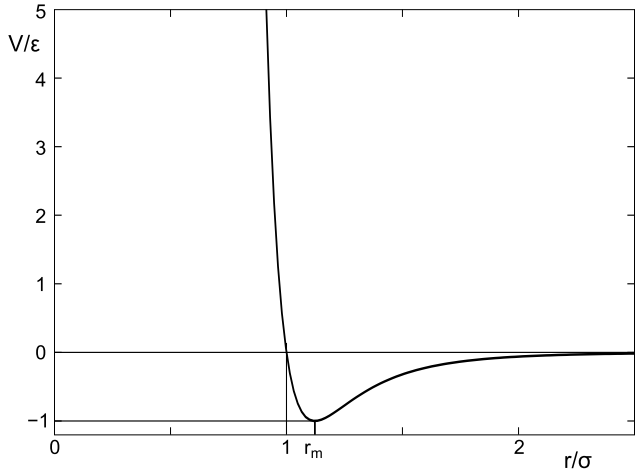


Figure 4: The Lennard–Jones potential. Make sure you label and have units on all axes! Also make sure that labels etc. are legible and that, if you print in black and white, that you use different line styles when required to differentiate between curves. In MATLAB you can export any figure to an .eps file from File → Export... in the Figure window.

Problem 2

In the following we give an example of how to produce a table. Use the code for Table 1 as a template.

Problem 3

If you find some part of the code particularly interesting you may include it in the text, otherwise it should be included in the appedix. If you do want to include code the

Table 1: A dummy table

Col. 1	Col. 2	Col. 3
the	quick	brown
fox	jumps	over
the	lazy	dog

following commands will print the text directly, with no LaTeX commands executed:

```
% Hello world ten times in MATLAB
for i = 1 : 10
  fprintf('Hello world %d!\n',i);
end
```

```
# Hello world ten times in Python
for i in range(10):
  print 'Hello world %d!' % i
```

Problem 4

At some point it may be appropriate to include equations. It is done in the following way:

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{1}$$

Do number and reference all your equations.

Concluding discussion

Use your favourite flavor of LaTeX to compile the file:

```
xelatex template.tex
pdflatex template.tex
latex template.tex
```

should all work. If you use `pdflatex` or `xelatex`, included figures need to be in `pdf`, `jpg`, or `png` format. If you want to include eps figures, you can easily convert them to `pdf` using the command

```
ps2pdf -dEPSCrop figure.eps figure.pdf
```

References

[1] Leslie Lamport, *LaTeX: A Document Preparation System*. Addison Wesley, Massachusetts, 2nd Edition, 1994.

A Source Code

Include all source code here in the appendix. Keep the code formatting clean, use indentation, and comment your code to make it easy to understand. Also, break lines that are too long. (Keep them under 80 characters!)

A.1 Calculating pi using matlab: `pi.m`

```
% Generate random points inside a centered square of area 4
trials = 1e6;
x = 2*rand(trials,1) - 1;
y = 2*rand(trials,1) - 1;

% Distance of points to (0,0)
r = sqrt(x.^2 + y.^2);

% Fraction of points inside unit circle
frac_inside = sum(r < 1)/trials;

fprintf('Pi is approximately %.6f.\n', 4*frac_inside);
```

A.2 Calculating pi using python: `pi.py`

```
#!/usr/bin/env python

from pylab import *

# Generate random points inside a centered square of area 4
trials = 1e6
x = 2*rand(trials,1) - 1
y = 2*rand(trials,1) - 1

# Distance of points to (0,0)
r = sqrt(x**2 + y**2)

# Fraction of points inside unit circle
frac_inside = sum(r < 1)/trials

sys.stdout.write('Pi is approximately %.6f.\n' % (4*frac_inside))
```

A.3 Calculating pi using C: `pi.c`

```
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#include <math.h>

#define TRIALS 1e8

int main() {
  float* x = malloc(TRIALS*sizeof(float));
  float* y = malloc(TRIALS*sizeof(float));
  int inside = 0;

  /* Seed RNG with current time */
  srand((unsigned)time(NULL));

  /* Generate random points inside a centered square of area 4
     and count the proportion that falls within the unit circle. */
  int i;
  for (i = 0; i < TRIALS; i++) {
    x[i] = 2.0 * (rand()/(RAND_MAX+1.0)) - 1.0;
    y[i] = 2.0 * (rand()/(RAND_MAX+1.0)) - 1.0;
    if (sqrt(x[i]*x[i]+y[i]*y[i]) < 1.0) {
      inside++;
    }
  }

  free(x);
  free(y);

  printf("Pi is approximately %.6f.\n", 4.0*inside/TRIALS);

  return 0;
}
```