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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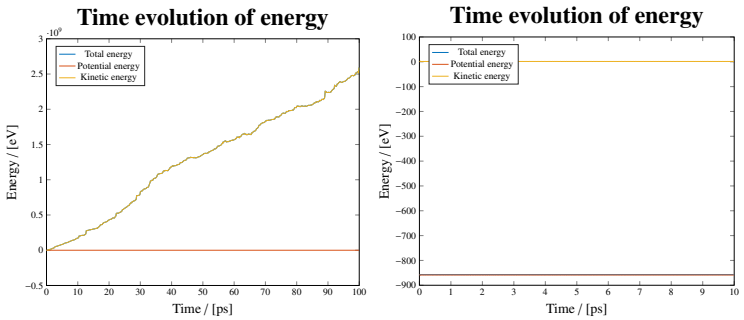
Task №	Points	Avail. points
Σ		

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

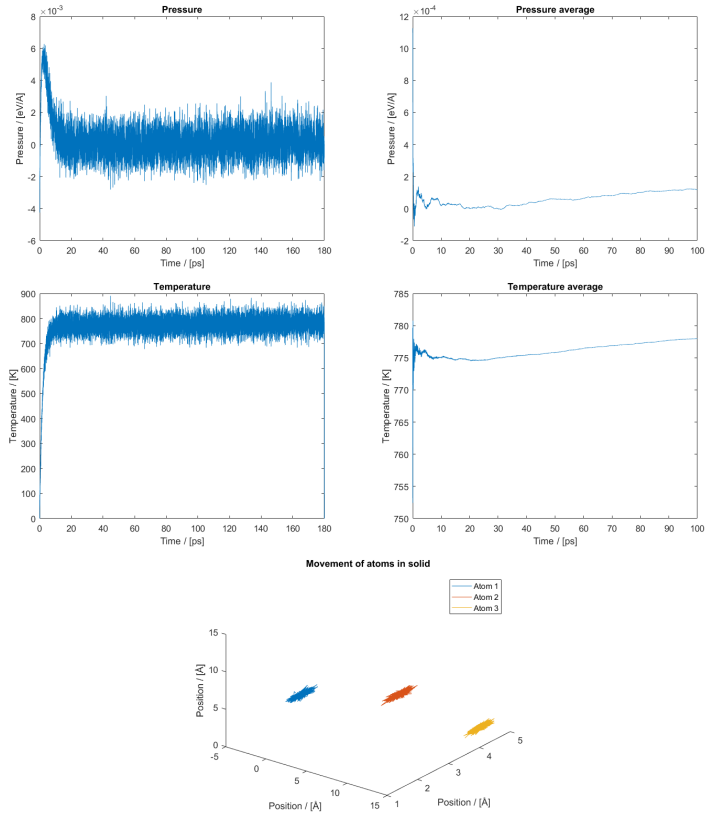


Figure 2: After the equilibrium, both the pressure and the temperature needs some time to stabilize after rescaling the velocities, but remains stable for longer time. The equalisation temperature was set to 500 C°.

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

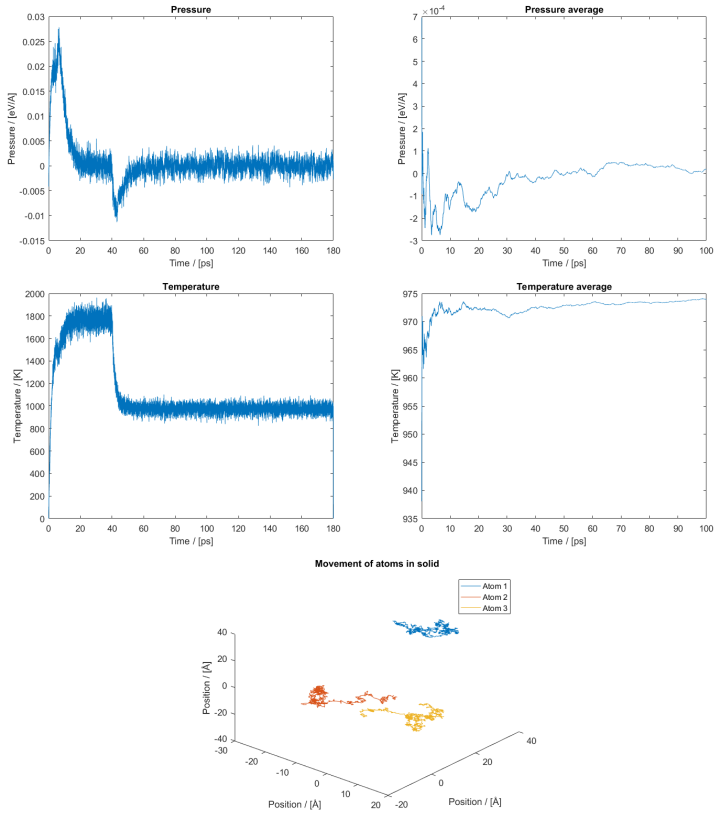


Figure 3: After the equilibrium, both the pressure and the temperature needs some time to stabilize after rescaling the velocities, but remains stable for longer time. The equalisation temperature was first set to 1000 C° for the smelting and then the temperature was reduced to 700 C°.

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 2.85 Å, which corresponds to the shortest distance in a fcc structure with the unit cell length of 4.046 Å. This is the distance between one of the corner atoms and a face centered atom close to that corner, which is expected. The other larger peaks are around 5 Å and 7.17 Å. These align with the two next shortest distances in an fcc structure.

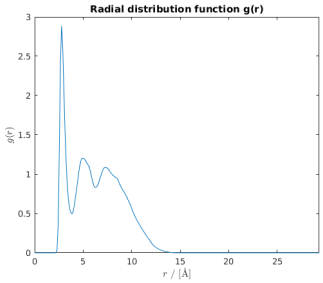


Figure 4: The radial function is computed by taking the histogram over all the internal distances between the atoms then divided by the random distribution of the same density.

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.

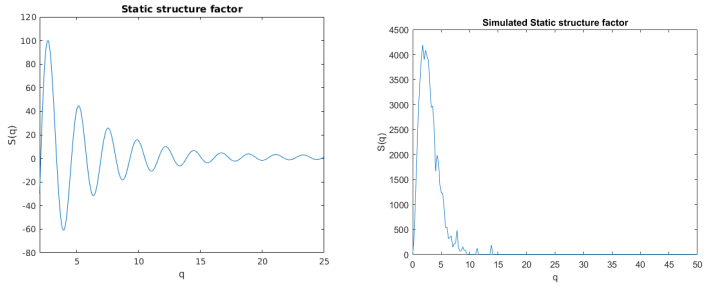


Figure 5: The static structure function computed both from the radial distribution function in figure 4 in the left and using bins in Fourier space to the right.

Concluding discussion

A Source code

A.1 Task1/MD_main.c

```c
/*
 MD_main.c

 Created by Anders Lindman on 2013-10-31.
 */

#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include <time.h>
#include "initfcc.h"
#include "alpotential.h"
#define nbr_of_particles 256
#define nbr_of_timesteps 1000
#define nbr_of_dimensions 3

double boundary_condition(double,double);


/* Main program */
int main()
{
    srand(time(NULL));

    /* Simulation parameters */
    double m_AL; // Mass of atom
    double cell_length; // Side length of supercell

    double lattice_spacing; // Smallest length between atoms
    double initial_displacement;    // Initial displacement of the atoms from their
                                    // lattice positions

    double lattice_param;   // Lattice parameter, length of each side in the
                            // unit cell

    double timestep;

    FILE *file1;
    FILE *file2;
    FILE *file3;


    /* Current displacement, velocities, and acceleratons */
    double q[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Displacements
    double v[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Velocities
    double f[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Forces

    /* Allocate memory for large vectors */
    /* Simulate 3 dimensional data by placing iniitalizeing a 1-dimensional array*/
    #define qq(i,j,k) (disp_arr[nbr_of_particles*nbr_of_dimensions*i+nbr_of_dimensions*j+k])
    double* disp_arr =(double*)malloc(nbr_of_timesteps*nbr_of_particles*nbr_of_dimensions*sizeof(double));

    double* energy =(double*)malloc(nbr_of_timesteps*sizeof(double));
    double* energy_kin = (double*)malloc(nbr_of_timesteps*sizeof(double));
    double* virial =(double*)malloc(nbr_of_timesteps*sizeof(double));

    //TODO go over parameters again
    /* Initialize parameters*/
    initial_displacement = 0.05;
    lattice_param = 4.046; // For aluminium (  )
    lattice_spacing = lattice_param/sqrt(2.0);
    timestep = 0.01; // 0.1 Bad, 0.01 Seems decent
    m_AL = 0.0027964; // In ASU
    cell_length = 4*lattice_param;  // Side of the supercell: The 256 atoms are
                                    // structured in a block of 4x4x4 unit cells

    // Initialize all displacements, for all times, as 0
    for (int i  = 0; i < nbr_of_timesteps; i++){
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                qq(i,j,k) = 0;
            }
        }
    }

    /* Put atoms on lattice */
```

```
77      init_fcc(q, 4, lattice_param);
78
79      /* Initial conditions */
80
81      for (int i = 0; i < nbr_of_particles; i++){
82          for (int j = 0; j < nbr_of_dimensions; j++){
83
84              // Initial perturbation from equilibrium
85              q[i][j] +=lattice_spacing* initial_displacement
86                  * ((double)rand()/(double)RAND_MAX);
87
88          }
89      }
90
91
92      for (int i = 0; i < nbr_of_particles; i++){
93          for (int j = 0; j < nbr_of_dimensions; j++){
94              qq(0,i,j)=q[i][j];
95          }
96      }
97
98      energy[0]=get_energy_AL(q,cell_length,nbr_of_particles);
99      virial[0]=get_virial_AL(q,cell_length,nbr_of_particles);
100     energy_kin[0]=get_kinetic_AL(v,nbr_of_dimensions,nbr_of_particles,m_AL);
101
102     get_forces_AL(f,q,cell_length,nbr_of_particles);
103
104
105     /* Simulation */
106     for (int i = 1; i < nbr_of_timesteps; i++)
107     {
108         /** Verlet algorithm **/
109         /* Half step for velocity */
110         for (int j = 0; j < nbr_of_particles; j++){
111             for (int k = 0; k < nbr_of_dimensions; k++){
112                 v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
113             }
114         }
115
116         /* Update displacement*/
117         for (int j = 0; j < nbr_of_particles; j++){
118             for (int k = 0; k < nbr_of_dimensions; k++){
119                 q[j][k] += timestep * v[j][k];
120             }
121         }
122
123         /* Forces */
124         get_forces_AL(f,q,cell_length,nbr_of_particles);
125
126         /* Final velocity*/
127         for (int j = 0; j < nbr_of_particles; j++){
128             for (int k = 0; k < nbr_of_dimensions; k++){
129                 v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
130             }
131         }
132
133         /* Calculate energy */
134         // Potential energy
135         energy[i] = get_energy_AL(q,cell_length,nbr_of_particles);
136         // Kinetic energy
137         energy_kin[i] = get_kinetic_AL(v,nbr_of_dimensions,nbr_of_particles,m_AL↩
                );
138
139         virial[i]=get_virial_AL(q,cell_length,nbr_of_particles);
140
141         /* Save current displacements to array*/
142         for (int j = 0; j < nbr_of_particles; j++){
143             for (int k = 0; k < nbr_of_dimensions; k++){
144                 qq(i,j,k)=q[j][k];
145             }
146         }
147     }
148
149     /* Save data to file*/
150     file1 = fopen("displacement.dat","w");
151
152     double current_time;
153     for (int i = 0; i < nbr_of_timesteps; i ++)
154     {
155         current_time = i*timestep;
156         fprintf(file1, "%.4f \t", current_time );
157         for (int j = 0; j < nbr_of_particles; j++)
158         {
159             for (int k = 0; k < nbr_of_dimensions; k++)
160             {
161                 fprintf(file1, "%.4f \t", qq(i,j,k));
162             }
163         }
164         fprintf(file1, "\n");
165     }
166     fclose(file1);
```

```
167
168     /* Save energies to file */
169     file2 = fopen("energy.dat","w");
170
171     for (int i = 0; i < nbr_of_timesteps; i ++)
172     {
173         current_time = i*timestep;
174         fprintf(file2, "%.4f \t", current_time);
175         fprintf(file2, "%.4f \t", energy[i]);
176         fprintf(file2, "%.4f \n", energy_kin[i]);
177     }
178     fclose(file2);
179
180     /* Save energies to file */
181     file3 = fopen("virial.dat","w");
182
183     for (int i = 0; i < nbr_of_timesteps; i ++)
184     {
185         current_time = i*timestep;
186         fprintf(file3, "%.4f \t", current_time);
187         fprintf(file3, "%.4f \n", virial[i]);
188     }
189     fclose(file3);
190
191     free(energy_kin); energy_kin=NULL;
192     free(energy); energy=NULL;
193     free(disp_arr); disp_arr=NULL;
194     free(virial); virial=NULL;
195
196     return 0;
197 }
198
199
200 double boundary_condition(double u, double L)
201 {
202
203     double f = fmod(u,L);
204     if (f < 0)
205         return -f;
206     else
207         return f;
208 }
```

A.2 Task3/MD_main.c

```
1
2
3  #include <stdio.h>
4  #include <math.h>
5  #include <stdlib.h>
6  #include <time.h>
7  #include "initfcc.h"
8  #include "alpotential.h"
9  #define nbr_of_particles 256
10 #define nbr_of_timesteps 1e4
11 #define nbr_of_timesteps_eq 4000
12 #define nbr_of_dimensions 3
13
14 double boundary_condition(double,double);
15
16
17
18 /* Main program */
19 int main()
20 {
21     srand(time(NULL));
22
23     /* Simulation parameters */
24     double m_AL; // Mass of atom
25     double cell_length; // Side length of supercell
26     double volume;
27     double lattice_spacing; // Smallest length between atoms
28     double initial_displacement;    // Initial displacement of the atoms from ↩
           their
29                                     // lattice positions
30     double lattice_param;   // Lattice parameter, length of each side in the
31                             // unit cell
32     double timestep;
33     double temperature_eq[] = { 500.0+273.15, 500.0+273.15 };
34     double pressure_eq = 101325e-11/1.602; // 1 atm in ASU
35
36     FILE *file;
37
38
39     /* Current displacement, velocities, and acceleratons */
40     double q[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Displacements
```

```
    double v[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Velocities
    double f[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Forces

    /* Allocate memory for large vectors */
    /* Simulate 3 dimensional data by placing iniitalizeing a 1-dimensional array*/
    #define qq(i,j,k) (disp_arr[nbr_of_particles*nbr_of_dimensions*i+nbr_of_dimensions*j+k])
    double* disp_arr = (double*)malloc(nbr_of_timesteps*nbr_of_particles*nbr_of_dimensions*sizeof(double));

    double* energy          = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* energy_kin      = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* virial          = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* temperature_avg = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* pressure_avg    = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* temperature     = (double*) malloc((2 * nbr_of_timesteps_eq + nbr_of_timesteps) * sizeof(double));
    double* pressure        = (double*) malloc((2 * nbr_of_timesteps_eq + nbr_of_timesteps) * sizeof(double));

    //TODO go over parameters again
    /* Initialize parameters*/
    initial_displacement    = 0.05;
    lattice_param           = 4.046; // For aluminium (  )
    lattice_spacing         = lattice_param/sqrt(2.0);
    timestep                = 0.01; // 0.1 Bad, 0.01 Seems decent
    m_AL                    = 0.0027964; // In ASU
    cell_length             = 4*lattice_param;  // Side of the supercell: The 256 atoms are
                                                // structured in a block of 4x4x4 unit cells
    volume                  = pow(cell_length, 3);

    // Initialize all displacements, for all times, as 0
    for (int i  = 0; i < nbr_of_timesteps; i++){
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                qq(i,j,k) = 0;
            }
        }
    }

    /* Put atoms on lattice */
    init_fcc(q, 4, lattice_param);


    /* Initial conditions */
    for (int i = 0; i < nbr_of_particles; i++){
        for (int j = 0; j < nbr_of_dimensions; j++){

            // Initial perturbation from equilibrium
            q[i][j] += lattice_spacing * initial_displacement
                * ((double)rand()/(double)RAND_MAX);

        }
    }


    get_forces_AL(f, q, cell_length, nbr_of_particles);

    /* Simulation */
    /* Equilibrium stage */

    double inst_temperature_eq;
    double inst_pressure_eq;
    double alpha_T = 1.0;
    double alpha_P = 1.0;
    double energy_kin_eq = get_kinetic_AL(v,nbr_of_dimensions,nbr_of_particles,m_AL);
    double virial_eq = get_virial_AL(q,cell_length,nbr_of_particles);

    temperature[0]  = instantaneous_temperature(energy_kin_eq, nbr_of_particles);
    pressure[0]     = instantaneous_pressure(virial_eq, temperature[0], nbr_of_particles, volume);

    for (int equil = 0; equil < 2; equil++) {
        for (int i = 1; i < nbr_of_timesteps_eq; i++)
        {
            /** Verlet algorithm **/
            /* Half step for velocity */
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
                }
```

```
            }

            /* Update displacement*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    q[j][k] += timestep * v[j][k];
                }
            }

            /* Forces */
            get_forces_AL(f,q,cell_length,nbr_of_particles);

            /* Final velocity*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] += timestep * 0.5* f[j][k]/m_AL;
                }
            }

            /* Calculate energy */
            // Kinetic energy
            energy_kin_eq = get_kinetic_AL(v, nbr_of_dimensions, ↩
                 nbr_of_particles, m_AL);

            virial_eq = get_virial_AL(q, cell_length, nbr_of_particles);


            inst_temperature_eq = instantaneous_temperature(energy_kin_eq, ↩
                 nbr_of_particles);
            temperature[equil*(nbr_of_timesteps_eq-1) + i] = inst_temperature_eq↩
                 ;
            inst_pressure_eq = instantaneous_pressure(virial_eq, ↩
                 inst_temperature_eq,
                nbr_of_particles, volume);
            pressure[equil*(nbr_of_timesteps_eq-1) + i] = inst_pressure_eq;


            // Update alhpas
            alpha_T = 1.0 + 0.01*(temperature_eq[equil]-inst_temperature_eq)/↩
                 inst_temperature_eq;
            alpha_P = 1.0 - 0.01*(pressure_eq - inst_pressure_eq);


            // Scale velocities
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] *= sqrt(alpha_T);
                }
            }

            // Scale positions and volume
            cell_length *= pow(alpha_P, 1.0/3.0);
            volume = pow(cell_length, 3);
            for (int j = 0; j < nbr_of_particles; j++) {
                for (int k = 0; k < nbr_of_dimensions; k++) {
                    q[j][k] *= pow(alpha_P, 1.0/3.0);
                }
            }

        }
    }

    printf("Equilibration done.\n");
    printf("Cell length: %.8f \n", cell_length);

    for (int i = 0; i < nbr_of_particles; i++){
        for (int j = 0; j < nbr_of_dimensions; j++){
            qq(0,i,j)=q[i][j];
        }
    }

    // Compute energies, temperature etc. at equilibrium
    energy[0] = get_energy_AL(q, cell_length, nbr_of_particles);
    virial[0] = get_virial_AL(q, cell_length, nbr_of_particles);
    energy_kin[0] = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles, m_AL)↩
         ;
    temperature_avg[0] = instantaneous_temperature(energy_kin[0], ↩
         nbr_of_particles);
    pressure_avg[0] = instantaneous_pressure(virial[0], temperature_avg[0],
        nbr_of_particles, volume);

    /* Simulation after equilibrium*/
    for (int i = 1; i < nbr_of_timesteps; i++)
    {
        /** Verlet algorithm **/
        /* Half step for velocity */
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
            }
        }
```

```
201
202         /* Update displacement*/
203         for (int j = 0; j < nbr_of_particles; j++){
204             for (int k = 0; k < nbr_of_dimensions; k++){
205                 q[j][k] += timestep * v[j][k];
206             }
207         }
208
209         /* Update Forces */
210         get_forces_AL(f, q, cell_length, nbr_of_particles);
211
212         /* Final velocity*/
213         for (int j = 0; j < nbr_of_particles; j++){
214             for (int k = 0; k < nbr_of_dimensions; k++){
215                 v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
216             }
217         }
218
219         /* Calculate energy */
220         // Potential energy
221         energy[i] = get_energy_AL(q, cell_length, nbr_of_particles);
222         // Kinetic energy
223         energy_kin[i] = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles, ↩
                m_AL);
224
225         virial[i] = get_virial_AL(q, cell_length, nbr_of_particles);
226
227         // Temperature
228         temperature_avg[i] = averaged_temperature(energy_kin, nbr_of_particles, ↩
                i);
229         temperature[2*(nbr_of_timesteps_eq-1) + i] = instantaneous_temperature(↩
                energy_kin[i],
230             nbr_of_particles);
231
232
233         // Pressure
234         pressure_avg[i] = averaged_pressure(virial, energy_kin, volume, i);
235         pressure[2*(nbr_of_timesteps_eq-1) + i] = instantaneous_pressure(virial[↩
                i],
236             temperature[2*(nbr_of_timesteps_eq-1) + i],
237             nbr_of_particles, volume);
238
239
240         /* Save current displacements to array*/
241         for (int j = 0; j < nbr_of_particles; j++){
242             for (int k = 0; k < nbr_of_dimensions; k++){
243                 qq(i,j,k)=q[j][k];
244             }
245         }
246
247     } // equilibration/simulation
248
249     /* Save data to file*/
250     file = fopen("displacement.dat","w");
251
252     double current_time;
253     for (int i = 0; i < nbr_of_timesteps; i ++) {
254         current_time = i*timestep;
255         fprintf(file, "%.4f \t", current_time );
256         for (int j = 0; j < nbr_of_particles; j++) {
257             for (int k = 0; k < nbr_of_dimensions; k++) {
258                 fprintf(file, "%.4f \t", qq(i,j,k));
259             }
260         }
261         fprintf(file, "\n");
262     }
263     fclose(file);
264
265     /* Save energies to file */
266     file = fopen("energy.dat","w");
267
268     for (int i = 0; i < nbr_of_timesteps; i ++) {
269         current_time = i*timestep;
270         fprintf(file, "%.4f \t", current_time);
271         fprintf(file, "%.4f \t", energy[i]);
272         fprintf(file, "%.4f \n", energy_kin[i]);
273     }
274     fclose(file);
275
276     // Save temperature to file
277     file = fopen("temperature.dat", "w");
278     for (int i = 0; i < 2*nbr_of_timesteps_eq+nbr_of_timesteps; i++) {
279         current_time = i*timestep;
280         fprintf(file, "%.3f \t %e\n", current_time, temperature[i]);
281     }
282     fclose(file);
283
284     file = fopen("temperature_avg.dat", "w");
285     for (int i = 0; i < nbr_of_timesteps; i++) {
286         current_time = i*timestep;
287         fprintf(file, "%.3f \t %e\n", current_time, temperature_avg[i]);
```

```
    }
    fclose(file);

    // Save pressure to file
    file = fopen("pressure.dat", "w");
    for (int i = 0; i < 2*nbr_of_timesteps_eq+nbr_of_timesteps; i++) {
        current_time = i*timestep;
        fprintf(file, "%.3f \t%e \n", current_time, pressure[i]);
    }
    fclose(file);

    file = fopen("pressure_avg.dat", "w");
    for (int i = 0; i < nbr_of_timesteps; i++) {
        current_time = i*timestep;
        fprintf(file, "%.3f \t %e\n", current_time, pressure_avg[i]);
    }
    fclose(file);


    free(energy_kin);       energy_kin = NULL;
    free(energy);           energy = NULL;
    free(disp_arr);         disp_arr = NULL;
    free(virial);           virial = NULL;
    free(temperature_avg);  temperature_avg = NULL;
    free(pressure_avg);     pressure_avg = NULL;
    free(temperature);      temperature = NULL;
    free(pressure);         pressure = NULL;

    return 0;
}
```

A.3 Task4/MD_main.c

```


#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include <time.h>
#include "initfcc.h"
#include "alpotential.h"
#define nbr_of_particles 256
#define nbr_of_timesteps 1e4
#define nbr_of_timesteps_eq 4000
#define nbr_of_dimensions 3

double boundary_condition(double,double);



/* Main program */
int main()
{
    srand(time(NULL));

    /* Simulation parameters */
    double m_AL; // Mass of atom
    double cell_length; // Side length of supercell
    double volume;
    double lattice_spacing; // Smallest length between atoms
    double initial_displacement;    // Initial displacement of the atoms from ↩
        their
                                    // lattice positions
    double lattice_param;   // Lattice parameter, length of each side in the
                            // unit cell
    double timestep;
    double temperature_eq[] = { 1500.0+273.15, 700.0+273.15 };
    double pressure_eq = 101325e-11/1.602; // 1 atm in ASU

    FILE *file;


    /* Current displacement, velocities, and acceleratons */
    double q[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Displacements
    double v[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Velocities
    double f[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Forces

    /* Allocate memory for large vectors */
    /* Simulate 3 dimensional data by placing iniitalizeing a 1-dimensional ↩
        array*/
    #define qq(i,j,k) (disp_arr[nbr_of_particles*nbr_of_dimensions*i+↩
        nbr_of_dimensions*j+k])
    double* disp_arr = (double*)malloc(nbr_of_timesteps*nbr_of_particles*↩
        nbr_of_dimensions*sizeof(double));

```

```
    double* energy          = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* energy_kin      = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* virial          = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* temperature_avg = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* pressure_avg    = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* temperature     = (double*) malloc((2 * nbr_of_timesteps_eq + nbr_of_timesteps) * sizeof(double));
    double* pressure        = (double*) malloc((2 * nbr_of_timesteps_eq + nbr_of_timesteps) * sizeof(double));

    //TODO go over parameters again
    /* Initialize parameters*/
    initial_displacement    = 0.05;
    lattice_param           = 4.046; // For aluminium (  )
    lattice_spacing         = lattice_param/sqrt(2.0);
    timestep                = 0.01; // 0.1 Bad, 0.01 Seems decent
    m_AL                    = 0.0027964; // In ASU
    cell_length             = 4*lattice_param;  // Side of the supercell: The 256 atoms are
                                                // structured in a block of 4x4x4 unit cells
    volume                  = pow(cell_length, 3);

    // Initialize all displacements, for all times, as 0
    for (int i  = 0; i < nbr_of_timesteps; i++){
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                qq(i,j,k) = 0;
            }
        }
    }

    /* Put atoms on lattice */
    init_fcc(q, 4, lattice_param);


    /* Initial conditions */
    for (int i = 0; i < nbr_of_particles; i++){
        for (int j = 0; j < nbr_of_dimensions; j++){

            // Initial perturbation from equilibrium
            q[i][j] += lattice_spacing * initial_displacement
                * ((double)rand()/(double)RAND_MAX);

        }
    }


    get_forces_AL(f, q, cell_length, nbr_of_particles);

    /* Simulation */
    /* Equilibrium stage */

    double inst_temperature_eq;
    double inst_pressure_eq;
    double alpha_T = 1.0;
    double alpha_P = 1.0;
    double energy_kin_eq = get_kinetic_AL(v,nbr_of_dimensions,nbr_of_particles,m_AL);
    double virial_eq = get_virial_AL(q,cell_length,nbr_of_particles);

    temperature[0]  = instantaneous_temperature(energy_kin_eq, nbr_of_particles);
    pressure[0]     = instantaneous_pressure(virial_eq, temperature[0], nbr_of_particles, volume);

    for (int equil = 0; equil < 2; equil++) {
        for (int i = 1; i < nbr_of_timesteps_eq; i++)
        {
            /** Verlet algorithm **/
            /* Half step for velocity */
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
                }
            }

            /* Update displacement*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    q[j][k] += timestep * v[j][k];
                }
            }

            /* Forces */
            get_forces_AL(f,q,cell_length,nbr_of_particles);
```

```
            /* Final velocity*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] += timestep * 0.5* f[j][k]/m_AL;
                }
            }

            /* Calculate energy */
            // Kinetic energy
            energy_kin_eq = get_kinetic_AL(v, nbr_of_dimensions, ↩
                 nbr_of_particles, m_AL);

            virial_eq = get_virial_AL(q, cell_length, nbr_of_particles);


            inst_temperature_eq = instantaneous_temperature(energy_kin_eq, ↩
                 nbr_of_particles);
            temperature[equil*(nbr_of_timesteps_eq-1) + i] = inst_temperature_eq↩
                 ;
            inst_pressure_eq = instantaneous_pressure(virial_eq, ↩
                 inst_temperature_eq,
                nbr_of_particles, volume);
            pressure[equil*(nbr_of_timesteps_eq-1) + i] = inst_pressure_eq;


            // Update alhpas
            alpha_T = 1.0 + 0.01*(temperature_eq[equil]-inst_temperature_eq)/↩
                 inst_temperature_eq;
            alpha_P = 1.0 - 0.01*(pressure_eq - inst_pressure_eq);


            // Scale velocities
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] *= sqrt(alpha_T);
                }
            }

            // Scale positions and volume
            cell_length *= pow(alpha_P, 1.0/3.0);
            volume = pow(cell_length, 3);
            for (int j = 0; j < nbr_of_particles; j++) {
                for (int k = 0; k < nbr_of_dimensions; k++) {
                    q[j][k] *= pow(alpha_P, 1.0/3.0);
                }
            }

        }
    }

    printf("Equilibration done.\n");
    printf("Cell length: %.8f \n", cell_length);

    for (int i = 0; i < nbr_of_particles; i++){
        for (int j = 0; j < nbr_of_dimensions; j++){
            qq(0,i,j)=q[i][j];
        }
    }

    // Compute energies, temperature etc. at equilibrium
    energy[0] = get_energy_AL(q, cell_length, nbr_of_particles);
    virial[0] = get_virial_AL(q, cell_length, nbr_of_particles);
    energy_kin[0] = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles, m_AL)↩
         ;
    temperature_avg[0] = instantaneous_temperature(energy_kin[0], ↩
         nbr_of_particles);
    pressure_avg[0] = instantaneous_pressure(virial[0], temperature_avg[0],
        nbr_of_particles, volume);

    /* Simulation after equilibrium*/
    for (int i = 1; i < nbr_of_timesteps; i++)
    {
        /** Verlet algorithm **/
        /* Half step for velocity */
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
            }
        }

        /* Update displacement*/
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                q[j][k] += timestep * v[j][k];
            }
        }

        /* Update Forces */
        get_forces_AL(f, q, cell_length, nbr_of_particles);
```

```
212         /* Final velocity*/
213         for (int j = 0; j < nbr_of_particles; j++){
214             for (int k = 0; k < nbr_of_dimensions; k++){
215                 v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
216             }
217         }
218 
219         /* Calculate energy */
220         // Potential energy
221         energy[i] = get_energy_AL(q, cell_length, nbr_of_particles);
222         // Kinetic energy
223         energy_kin[i] = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles, ↩
                m_AL);
224 
225         virial[i] = get_virial_AL(q, cell_length, nbr_of_particles);
226 
227         // Temperature
228         temperature_avg[i] = averaged_temperature(energy_kin, nbr_of_particles, ↩
                i);
229         temperature[2*(nbr_of_timesteps_eq-1) + i] = instantaneous_temperature(↩
                energy_kin[i],
230             nbr_of_particles);
231 
232 
233         // Pressure
234         pressure_avg[i] = averaged_pressure(virial, energy_kin, volume, i);
235         pressure[2*(nbr_of_timesteps_eq-1) + i] = instantaneous_pressure(virial[↩
                i],
236             temperature[2*(nbr_of_timesteps_eq-1) + i],
237             nbr_of_particles, volume);
238 
239 
240         /* Save current displacements to array*/
241         for (int j = 0; j < nbr_of_particles; j++){
242             for (int k = 0; k < nbr_of_dimensions; k++){
243                 qq(i,j,k)=q[j][k];
244             }
245         }
246 
247     } // equilibration/simulation
248 
249     /* Save data to file*/
250     file = fopen("displacement.dat","w");
251 
252     double current_time;
253     for (int i = 0; i < nbr_of_timesteps; i ++) {
254         current_time = i*timestep;
255         fprintf(file, "%.4f \t", current_time );
256         for (int j = 0; j < nbr_of_particles; j++) {
257             for (int k = 0; k < nbr_of_dimensions; k++) {
258                 fprintf(file, "%.4f \t", qq(i,j,k));
259             }
260         }
261         fprintf(file, "\n");
262     }
263     fclose(file);
264 
265     /* Save energies to file */
266     file = fopen("energy.dat","w");
267 
268     for (int i = 0; i < nbr_of_timesteps; i ++) {
269         current_time = i*timestep;
270         fprintf(file, "%.4f \t", current_time);
271         fprintf(file, "%.4f \t", energy[i]);
272         fprintf(file, "%.4f \n", energy_kin[i]);
273     }
274     fclose(file);
275 
276     // Save temperature to file
277     file = fopen("temperature.dat", "w");
278     for (int i = 0; i < 2*nbr_of_timesteps_eq+nbr_of_timesteps; i++) {
279         current_time = i*timestep;
280         fprintf(file, "%.3f \t %e\n", current_time, temperature[i]);
281     }
282     fclose(file);
283 
284     file = fopen("temperature_avg.dat", "w");
285     for (int i = 0; i < nbr_of_timesteps; i++) {
286         current_time = i*timestep;
287         fprintf(file, "%.3f \t %e\n", current_time, temperature_avg[i]);
288     }
289     fclose(file);
290 
291     // Save pressure to file
292     file = fopen("pressure.dat", "w");
293     for (int i = 0; i < 2*nbr_of_timesteps_eq+nbr_of_timesteps; i++) {
294         current_time = i*timestep;
295         fprintf(file, "%.3f \t%e \n", current_time, pressure[i]);
296     }
297     fclose(file);
298 
```

```
    file = fopen("pressure_avg.dat", "w");
    for (int i = 0; i < nbr_of_timesteps; i++) {
        current_time = i*timestep;
        fprintf(file, "%.3f \t %e\n", current_time, pressure_avg[i]);
    }
    fclose(file);


    free(energy_kin);       energy_kin = NULL;
    free(energy);           energy = NULL;
    free(disp_arr);         disp_arr = NULL;
    free(virial);           virial = NULL;
    free(temperature_avg);  temperature_avg = NULL;
    free(pressure_avg);     pressure_avg = NULL;
    free(temperature);      temperature = NULL;
    free(pressure);         pressure = NULL;

    return 0;
}
```

A.4 Task5/MD_main.c

```
/*
 MD_main.c

 Created by Anders Lindman on 2013-10-31.
 */

#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include <time.h>
#include "initfcc.h"
#include "alpotential.h"
#define nbr_of_particles 256
#define nbr_of_timesteps 1e4
#define nbr_of_timesteps_eq 4000
#define nbr_of_dimensions 3

double boundary_condition(double,double);



/* Main program */
int main()
{
    srand(time(NULL));

    /* Simulation parameters */
    double m_AL; // Mass of atom
    double cell_length; // Side length of supercell
    double volume;
    double lattice_spacing; // Smallest length between atoms
    double initial_displacement;    // Initial displacement of the atoms from ↩
        their
                                    // lattice positions
    double lattice_param;   // Lattice parameter, length of each side in the
                            // unit cell
    double timestep;
    double temperature_eq[] = { 1000.0+273.15, 700.0+273.15 };
    double pressure_eq = 101325e-11/1.602; // 1 atm in ASU
    double isothermal_compressibility = 1.0; //0.8645443196; // 1.385e-11 m^2/N ↩
        = 1.385/1.602    ^3/eV

    FILE *file;


    /* Current displacement, velocities, and acceleratons */
    double q[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Displacements
    double v[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Velocities
    double f[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Forces

    double heat_capacity_pot, heat_capacity_kin;

    /* Allocate memory for large vectors */
    /* Simulate 3 dimensional data by placing iniitalizeing a 1-dimensional ↩
        array*/
    #define qq(i,j,k) (disp_arr[nbr_of_particles*nbr_of_dimensions*i+↩
        nbr_of_dimensions*j+k])
    double* disp_arr = (double*)malloc(nbr_of_timesteps*nbr_of_particles*↩
        nbr_of_dimensions*sizeof(double));

    double* energy_pot      = (double*) malloc(nbr_of_timesteps * sizeof(double)↩
        );
    double* energy_kin      = (double*) malloc(nbr_of_timesteps * sizeof(double)↩
        );
```

```
    double* virial          = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* temperature_avg = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* pressure_avg    = (double*) malloc(nbr_of_timesteps * sizeof(double));
    //double* temperature     = (double*) malloc((2 * nbr_of_timesteps_eq + nbr_of_timesteps) * sizeof(double));
    //double* pressure        = (double*) malloc((2 * nbr_of_timesteps_eq + nbr_of_timesteps) * sizeof(double));

    //TODO go over parameters again
    /* Initialize parameters*/
    initial_displacement    = 0.05;
    lattice_param           = 4.046; // For aluminium (  )
    lattice_spacing         = lattice_param/sqrt(2.0);
    timestep                = 0.001; // 0.1 Bad, 0.01 Seems decent
    m_AL                    = 0.0027964; // In ASU
    cell_length             = 4*lattice_param;  // Side of the supercell: The 256 atoms are
                                                // structured in a block of 4x4x4 unit cells
    volume                  = pow(cell_length, 3);

    // Initialize all displacements, for all times, as 0
    for (int i  = 0; i < nbr_of_timesteps; i++){
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                qq(i,j,k) = 0;
            }
        }
    }

    /* Put atoms on lattice */
    init_fcc(q, 4, lattice_param);


    /* Initial conditions */
    for (int i = 0; i < nbr_of_particles; i++){
        for (int j = 0; j < nbr_of_dimensions; j++){

            // Initial perturbation from equilibrium
            q[i][j] += lattice_spacing * initial_displacement
                * ((double)rand()/(double)RAND_MAX);

        }
    }


    get_forces_AL(f, q, cell_length, nbr_of_particles);

    /* Simulation */
    /* Equilibrium stage */

    double inst_temperature_eq;
    double inst_pressure_eq;
    double alpha_T = 1.0;
    double alpha_P = 1.0;
    double energy_kin_eq = get_kinetic_AL(v,nbr_of_dimensions,nbr_of_particles,m_AL);
    double virial_eq = get_virial_AL(q,cell_length,nbr_of_particles);

    //temperature[0]  = instantaneous_temperature(energy_kin_eq, nbr_of_particles);
    //pressure[0]     = instantaneous_pressure(virial_eq, temperature[0], nbr_of_particles, volume);

    for (int equil = 0; equil < 2; equil++) {
        for (int i = 1; i < nbr_of_timesteps_eq; i++)
        {
            /** Verlet algorithm **/
            /* Half step for velocity */
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
                }
            }

            /* Update displacement*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    q[j][k] += timestep * v[j][k];
                }
            }

            /* Forces */
            get_forces_AL(f,q,cell_length,nbr_of_particles);

            /* Final velocity*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
```

```
                    v[j][k] += timestep * 0.5* f[j][k]/m_AL;
                }
            }

            /* Calculate energy */
            // Kinetic energy
            energy_kin_eq = get_kinetic_AL(v, nbr_of_dimensions, ↩
                nbr_of_particles, m_AL);

            virial_eq = get_virial_AL(q, cell_length, nbr_of_particles);


            inst_temperature_eq = instantaneous_temperature(energy_kin_eq, ↩
                nbr_of_particles);
            //temperature[equil*(nbr_of_timesteps_eq-1) + i] = ↩
                inst_temperature_eq;
            inst_pressure_eq = instantaneous_pressure(virial_eq, ↩
                inst_temperature_eq,
                nbr_of_particles, volume);
            //pressure[equil*(nbr_of_timesteps_eq-1) + i] = inst_pressure_eq;


            // Update alhpas
            alpha_T = 1.0 + 0.01*(temperature_eq[equil]-inst_temperature_eq)/↩
                inst_temperature_eq;
            alpha_P = 1.0 - 0.01*isothermal_compressibility*(pressure_eq - ↩
                inst_pressure_eq);

            // DEBUG:alpha
            //printf("%.8f \t %.8f \n", alpha_T, alpha_P);

            // Scale velocities
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] *= sqrt(alpha_T);
                }
            }

            // Scale positions and volume
            cell_length *= pow(alpha_P, 1.0/3.0);
            volume = pow(cell_length, 3);
            for (int j = 0; j < nbr_of_particles; j++) {
                for (int k = 0; k < nbr_of_dimensions; k++) {
                    q[j][k] *= pow(alpha_P, 1.0/3.0);
                }
            }

        }
    }

    printf("Equilibration done.\n");
    printf("Cell length: %.8f \n", cell_length);

    for (int i = 0; i < nbr_of_particles; i++){
        for (int j = 0; j < nbr_of_dimensions; j++){
            qq(0,i,j)=q[i][j];
        }
    }

    // Compute energies, temperature etc. at equilibrium
    energy_pot[0] = get_energy_AL(q, cell_length, nbr_of_particles);
    virial[0] = get_virial_AL(q, cell_length, nbr_of_particles);
    energy_kin[0] = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles, m_AL)↩
        ;
    temperature_avg[0] = instantaneous_temperature(energy_kin[0], ↩
        nbr_of_particles);
    pressure_avg[0] = instantaneous_pressure(virial[0], temperature_avg[0],
        nbr_of_particles, volume);

    /* Simulation after equilibrium*/
    for (int i = 1; i < nbr_of_timesteps; i++)
    {
        /** Verlet algorithm **/
        /* Half step for velocity */
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
            }
        }

        /* Update displacement*/
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                q[j][k] += timestep * v[j][k];
            }
        }

        /* Update Forces */
        get_forces_AL(f, q, cell_length, nbr_of_particles);

        /* Final velocity*/
```

```
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
            }
        }

        /* Calculate energy */
        // Potential energy
        energy_pot[i] = get_energy_AL(q, cell_length, nbr_of_particles);
        // Kinetic energy
        energy_kin[i] = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles, ↩
             m_AL);

        virial[i] = get_virial_AL(q, cell_length, nbr_of_particles);

        // Temperature
        temperature_avg[i] = averaged_temperature(energy_kin, nbr_of_particles, ↩
             i);
        /*temperature[2*(nbr_of_timesteps_eq-1) + i] = instantaneous_temperature↩
             (energy_kin[i],
            nbr_of_particles);*/


        // Pressure
        pressure_avg[i] = averaged_pressure(virial, energy_kin, volume, i);
        /*pressure[2*(nbr_of_timesteps_eq-1) + i] = instantaneous_pressure(↩
             virial[i],
            temperature[2*(nbr_of_timesteps_eq-1) + i],
            nbr_of_particles, volume);*/


        /* Save current displacements to array*/
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                qq(i,j,k)=q[j][k];
            }
        }

    } // equilibration/simulation

    // Compute heat capacity
    heat_capacity_kin = calculate_heat_capacity_kin(energy_kin, temperature_eq↩
         [1],
        nbr_of_particles, nbr_of_timesteps);
    heat_capacity_pot = calculate_heat_capacity_pot(energy_pot, temperature_eq↩
         [1],
        nbr_of_particles, nbr_of_timesteps);

    printf("Temp: %f\nHeat capacity: %.10f \t %.10f\n", temperature_eq[1],
        heat_capacity_kin, heat_capacity_pot);

    // Save results to file
    file = fopen("heat_capacity.dat", "w");
    fprintf(file, "%.2f\t%e\t%e\n", temperature_eq[1],
        heat_capacity_kin, heat_capacity_pot);
    fclose(file);



    free(energy_kin);       energy_kin = NULL;
    free(energy_pot);       energy_pot = NULL;
    free(disp_arr);         disp_arr = NULL;
    free(virial);           virial = NULL;
    free(temperature_avg);  temperature_avg = NULL;
    free(pressure_avg);     pressure_avg = NULL;
    //free(temperature);        temperature = NULL;
    //free(pressure);           pressure = NULL;

    return 0;
}
```

A.5 Task6/MD_main.c

```
/*
 MD_main.c

 Created by Anders Lindman on 2013-10-31.
 */

#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include <time.h>
#include "initfcc.h"
#include "alpotential.h"
#define nbr_of_particles 256
```

```c
#define nbr_of_timesteps 1e4
#define nbr_of_timesteps_eq 4000
#define nbr_of_dimensions 3

double boundary_condition(double,double);



/* Main program */
int main()
{
    srand(time(NULL));

    /* Simulation parameters */
    double m_AL; // Mass of atom
    double cell_length; // Side length of supercell
    double volume;
    double lattice_spacing; // Smallest length between atoms
    double initial_displacement;    // Initial displacement of the atoms from their
                                    // lattice positions
    double lattice_param;   // Lattice parameter, length of each side in the
                            // unit cell
    double timestep;
    double temperature_eq[] = { 1000.0+273.15, 700.0+273.15 };
    double delta_temperature[] = { -10.0, 10.0 };
    double pressure_eq = 101325e-11/1.602; // 1 atm in ASU

    FILE *file;


    /* Current displacement, velocities, and acceleratons */
    double q[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Displacements
    double v[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Velocities
    double f[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Forces

    double heat_capacity;
    double energy_avg[2] = { 0 };
    double temperature_avg[2] = { 0 };


    /* Allocate memory for large vectors */

    double* energy_pot      = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* energy_kin      = (double*) malloc(nbr_of_timesteps * sizeof(double));


    /* Initialize parameters*/
    initial_displacement    = 0.05;
    lattice_param           = 4.046; // For aluminium (  )
    lattice_spacing         = lattice_param/sqrt(2.0);
    timestep                = 0.001; // 0.1 Bad, 0.01 Seems decent
    m_AL                    = 0.0027964; // In ASU
    cell_length             = 4*lattice_param;  // Side of the supercell: The 256 atoms are
                                                // structured in a block of 4x4x4 unit cells
    volume                  = pow(cell_length, 3);



    /* Put atoms on lattice */
    init_fcc(q, 4, lattice_param);


    /* Initial conditions */
    for (int i = 0; i < nbr_of_particles; i++){
        for (int j = 0; j < nbr_of_dimensions; j++){

            // Initial perturbation from equilibrium
            q[i][j] += lattice_spacing * initial_displacement
                * ((double)rand()/(double)RAND_MAX);

        }
    }


    get_forces_AL(f, q, cell_length, nbr_of_particles);

    /* Simulation */
    /* Equilibrium stage */

    double inst_temperature_eq;
    double inst_pressure_eq;
    double alpha_T = 1.0;
    double alpha_P = 1.0;
    double energy_kin_eq = get_kinetic_AL(v,nbr_of_dimensions,nbr_of_particles,m_AL);
    double virial_eq = get_virial_AL(q,cell_length,nbr_of_particles);
```

```
99
100     for (int d = 0; d < 2; d++) {
101
102         for (int equil = 0; equil < 2; equil++) {
103
104             double target_temp = temperature_eq[equil] + delta_temperature[d];
105
106             for (int i = 1; i < nbr_of_timesteps_eq; i++)
107             {
108                 /** Verlet algorithm **/
109                 /* Half step for velocity */
110                 for (int j = 0; j < nbr_of_particles; j++){
111                     for (int k = 0; k < nbr_of_dimensions; k++){
112                         v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
113                     }
114                 }
115
116                 /* Update displacement*/
117                 for (int j = 0; j < nbr_of_particles; j++){
118                     for (int k = 0; k < nbr_of_dimensions; k++){
119                         q[j][k] += timestep * v[j][k];
120                     }
121                 }
122
123                 /* Forces */
124                 get_forces_AL(f,q,cell_length,nbr_of_particles);
125
126                 /* Final velocity*/
127                 for (int j = 0; j < nbr_of_particles; j++){
128                     for (int k = 0; k < nbr_of_dimensions; k++){
129                         v[j][k] += timestep * 0.5* f[j][k]/m_AL;
130                     }
131                 }
132
133                 /* Calculate energy */
134                 // Kinetic energy
135                 energy_kin_eq = get_kinetic_AL(v, nbr_of_dimensions, ↩
                        nbr_of_particles, m_AL);
136
137                 virial_eq = get_virial_AL(q, cell_length, nbr_of_particles);
138
139
140                 inst_temperature_eq = instantaneous_temperature(energy_kin_eq, ↩
                        nbr_of_particles);
141                 inst_pressure_eq = instantaneous_pressure(virial_eq, ↩
                        inst_temperature_eq,
142                     nbr_of_particles, volume);
143
144
145                 // Update alhpas
146                 alpha_T = 1.0 + 0.01*(target_temp-inst_temperature_eq)/↩
                        inst_temperature_eq;
147                 alpha_P = 1.0 - 0.01*(pressure_eq - inst_pressure_eq);
148
149                 // Scale velocities
150                 for (int j = 0; j < nbr_of_particles; j++){
151                     for (int k = 0; k < nbr_of_dimensions; k++){
152                         v[j][k] *= sqrt(alpha_T);
153                     }
154                 }
155
156                 // Scale positions and volume
157                 cell_length *= pow(alpha_P, 1.0/3.0);
158                 volume = pow(cell_length, 3);
159                 for (int j = 0; j < nbr_of_particles; j++) {
160                     for (int k = 0; k < nbr_of_dimensions; k++) {
161                         q[j][k] *= pow(alpha_P, 1.0/3.0);
162                     }
163                 }
164
165             }
166         }
167
168
169         // Compute energies, temperature etc. at equilibrium
170         energy_pot[0] = get_energy_AL(q, cell_length, nbr_of_particles);
171         energy_kin[0] = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles, ↩
                m_AL);
172
173
174         /* Simulation after equilibrium*/
175         for (int i = 1; i < nbr_of_timesteps; i++)
176         {
177             /** Verlet algorithm **/
178             /* Half step for velocity */
179             for (int j = 0; j < nbr_of_particles; j++){
180                 for (int k = 0; k < nbr_of_dimensions; k++){
181                     v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
182                 }
183             }
184
```

```
            /* Update displacement*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    q[j][k] += timestep * v[j][k];
                }
            }

            /* Update Forces */
            get_forces_AL(f, q, cell_length, nbr_of_particles);

            /* Final velocity*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
                }
            }

            /* Calculate energy */
            // Potential energy
            energy_pot[i] = get_energy_AL(q, cell_length, nbr_of_particles);
            // Kinetic energy
            energy_kin[i] = get_kinetic_AL(v, nbr_of_dimensions, ↩
                 nbr_of_particles, m_AL);


        } // equilibration/simulation

        // Compute heat capacity
        temperature_avg[d] = averaged_temperature(energy_kin, nbr_of_particles, ↩
             nbr_of_timesteps-1);
        // Compute average total energy
        for (int i = 0; i < nbr_of_timesteps; i++)
            energy_avg[d] += energy_pot[i] + energy_kin[i];
        energy_avg[d] /= nbr_of_timesteps;

        printf("Temp: %f\nAverage total energy: %.10f\n", temperature_avg[d], ↩
             energy_avg[d]);

    }

    // Compute heat capacity
    heat_capacity = (energy_avg[1]-energy_avg[0])/(temperature_avg[1]-↩
         temperature_avg[0]);

    printf("heat capacity: %f\n", heat_capacity);

    // Save results to file
    file = fopen("heat_capacity.dat", "w");
    fprintf(file, "%.2f\t%e\n", temperature_eq[1], heat_capacity);
    fclose(file);



    free(energy_kin);       energy_kin = NULL;
    free(energy_pot);       energy_pot = NULL;

    return 0;
}
```

A.6 Task7/MD_main.c

```
/*
 MD_main.c

 Created by Anders Lindman on 2013-10-31.
 */

#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include <time.h>
#include "initfcc.h"
#include "alpotential.h"
#define nbr_of_particles 256
#define nbr_of_timesteps 1000
#define nbr_of_timesteps_eq 4000
#define nbr_of_dimensions 3

#define PI 3.141592653589
int get_bin(double , double , double , double );

double boundary_condition_dist_sq(double u1[3], double u2[3], double L);

/* Main program */
int main()
{
```

```
26      srand(time(NULL));
27
28      /* Simulation parameters */
29      double m_AL; // Mass of atom
30      double cell_length; // Side length of supercell
31      double volume;
32      double lattice_spacing; // Smallest length between atoms
33      double initial_displacement;    // Initial displacement of the atoms from ↩
            their
34                                      // lattice positions
35      double lattice_param;   // Lattice parameter, length of each side in the
36                              // unit cell
37      double timestep;
38      double temperature_eq[] = { 1500.0+273.15, 700.0+273.15 };
39      double pressure_eq = 101325e-11/1.602; // 1 atm in ASU
40      double isothermal_compressibility = 1.0; //0.8645443196; // 1.385e-11 m^2/N ↩
            = 1.385/1.602    ^3/eV
41
42      FILE *file;
43
44
45      /* Current displacement, velocities, and acceleratons */
46      double q[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Displacements
47      double v[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Velocities
48      double f[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Forces
49
50      /* Allocate memory for large vectors */
51      /* Simulate 3 dimensional data by placing iniitalizeing a 1-dimensional ↩
            array*/
52      #define qq(i,j,k) (disp_arr[nbr_of_particles*nbr_of_dimensions*i+↩
            nbr_of_dimensions*j+k])
53      double* disp_arr = (double*)malloc(nbr_of_timesteps*nbr_of_particles*↩
            nbr_of_dimensions*sizeof(double));
54
55      double* energy          = (double*) malloc(nbr_of_timesteps * sizeof(double)↩
            );
56      double* energy_kin      = (double*) malloc(nbr_of_timesteps * sizeof(double)↩
            );
57      double* virial          = (double*) malloc(nbr_of_timesteps * sizeof(double)↩
            );
58      double* temperature_avg = (double*) malloc(nbr_of_timesteps * sizeof(double)↩
            );
59      double* pressure_avg    = (double*) malloc(nbr_of_timesteps * sizeof(double)↩
            );
60      double* temperature     = (double*) malloc((2 * nbr_of_timesteps_eq + ↩
            nbr_of_timesteps) * sizeof(double));
61      double* pressure        = (double*) malloc((2 * nbr_of_timesteps_eq + ↩
            nbr_of_timesteps) * sizeof(double));
62
63
64      int k_bins  = 250;
65
66      //TODO go over parameters again
67      /* Initialize parameters*/
68      initial_displacement    = 0.05;
69      lattice_param           = 4.046; // For aluminium (  )
70      lattice_spacing         = lattice_param/sqrt(2.0);
71      timestep                = 0.01; // 0.1 Bad, 0.01 Seems decent
72      m_AL                    = 0.0027964; // In ASU
73      cell_length             = 4*lattice_param;  // Side of the supercell: The ↩
            256 atoms are
74                                                  // structured in a block of 4↩
                                                        x4x4 unit cells
75      volume                  = pow(cell_length, 3);
76
77      // Initialize all displacements, for all times, as 0
78      for (int i  = 0; i < nbr_of_timesteps; i++) {
79          for (int j = 0; j < nbr_of_particles; j++) {
80              for (int k = 0; k < nbr_of_dimensions; k++) {
81                  qq(i,j,k) = 0;
82              }
83          }
84      }
85
86      /* Put atoms on lattice */
87      init_fcc(q, 4, lattice_param);
88
89
90      /* Initial conditions */
91      for (int i = 0; i < nbr_of_particles; i++) {
92          for (int j = 0; j < nbr_of_dimensions; j++) {
93
94              // Initial perturbation from equilibrium
95              q[i][j] += lattice_spacing * initial_displacement
96                  * ((double)rand()/(double)RAND_MAX);
97
98          }
99      }
100
101
102     get_forces_AL(f, q, cell_length, nbr_of_particles);
```

```
103
104     /* Simulation */
105     /* Equilibrium stage */
106
107     double inst_temperature_eq;
108     double inst_pressure_eq;
109     double alpha_T = 1.0;
110     double alpha_P = 1.0;
111     double energy_kin_eq = get_kinetic_AL(v,nbr_of_dimensions,nbr_of_particles,↩
            m_AL);
112     double virial_eq = get_virial_AL(q,cell_length,nbr_of_particles);
113
114     temperature[0]  = instantaneous_temperature(energy_kin_eq, nbr_of_particles)↩
            ;
115     pressure[0]     = instantaneous_pressure(virial_eq, temperature[0], ↩
            nbr_of_particles, volume);
116
117     for (int equil = 0; equil < 2; equil++) {
118         for (int i = 1; i < nbr_of_timesteps_eq; i++) {
119
120             /** Verlet algorithm **/
121             /* Half step for velocity */
122             for (int j = 0; j < nbr_of_particles; j++) {
123                 for (int k = 0; k < nbr_of_dimensions; k++) {
124                     v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
125                 }
126             }
127
128             /* Update displacement*/
129             for (int j = 0; j < nbr_of_particles; j++) {
130                 for (int k = 0; k < nbr_of_dimensions; k++) {
131                     q[j][k] += timestep * v[j][k];
132                 }
133             }
134
135             /* Forces */
136             get_forces_AL(f,q,cell_length,nbr_of_particles);
137
138             /* Final velocity*/
139             for (int j = 0; j < nbr_of_particles; j++) {
140                 for (int k = 0; k < nbr_of_dimensions; k++) {
141                     v[j][k] += timestep * 0.5* f[j][k]/m_AL;
142                 }
143             }
144
145             /* Calculate energy */
146             // Kinetic energy
147             energy_kin_eq = get_kinetic_AL(v, nbr_of_dimensions, ↩
                    nbr_of_particles, m_AL);
148
149             virial_eq = get_virial_AL(q, cell_length, nbr_of_particles);
150
151
152             inst_temperature_eq = instantaneous_temperature(energy_kin_eq, ↩
                    nbr_of_particles);
153             temperature[equil*(nbr_of_timesteps_eq-1) + i] = inst_temperature_eq↩
                    ;
154             inst_pressure_eq = instantaneous_pressure(virial_eq, ↩
                    inst_temperature_eq,
155                 nbr_of_particles, volume);
156             pressure[equil*(nbr_of_timesteps_eq-1) + i] = inst_pressure_eq;
157
158
159             // Update alhpas
160             alpha_T = 1.0 + 0.01*(temperature_eq[equil]-inst_temperature_eq)/↩
                    inst_temperature_eq;
161             alpha_P = 1.0 - 0.01*isothermal_compressibility*(pressure_eq - ↩
                    inst_pressure_eq);
162
163
164             // Scale velocities
165             for (int j = 0; j < nbr_of_particles; j++) {
166                 for (int k = 0; k < nbr_of_dimensions; k++) {
167                     v[j][k] *= sqrt(alpha_T);
168                 }
169             }
170
171             // Scale positions and volume
172             cell_length *= pow(alpha_P, 1.0/3.0);
173             volume = pow(cell_length, 3);
174             for (int j = 0; j < nbr_of_particles; j++) {
175                 for (int k = 0; k < nbr_of_dimensions; k++) {
176                     q[j][k] *= pow(alpha_P, 1.0/3.0);
177                 }
178             }
179
180         }
181     }
182
183     for (int i = 0; i < nbr_of_particles; i++) {
184         for (int j = 0; j < nbr_of_dimensions; j++) {
```

```
            qq(0,i,j)=q[i][j];
        }
    }


    // Compute energies, temperature etc. at equilibrium
    double min = 0.0;
    double max = sqrt(3*cell_length*cell_length);
    double d_r = (max-min)/(1.0*k_bins);
    int bins[k_bins];
    int* bins2 = (int*) malloc(k_bins * sizeof(int));

    for (int i = 0; i < k_bins; i++) {
        bins[i]=0;
        bins2[i]=0;
    }

    for (int i = 1; i < nbr_of_timesteps; i++)
    {
        /** Verlet algorithm **/
        /* Half step for velocity */
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
            }
        }

        /* Update displacement*/
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                q[j][k] += timestep * v[j][k];
            }
        }

        /* Forces */
        get_forces_AL(f,q,cell_length,nbr_of_particles);

        /* Final velocity*/
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
            }
        }

        /* Calculate energy */
        // Potential energy
        energy[i] = get_energy_AL(q,cell_length,nbr_of_particles);
        // Kinetic energy
        energy_kin[i] = get_kinetic_AL(v,nbr_of_dimensions,nbr_of_particles,m_AL↩
            );

        virial[i]=get_virial_AL(q,cell_length,nbr_of_particles);

        /* Save current displacements to array*/
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                qq(i,j,k)=q[j][k];
            }
        }
    }


    // Create Histogram

    for (int i = 1; i < nbr_of_timesteps; i++)
    {
        for (int j = 1 ; j < nbr_of_particles; j++) {
            for (int k = j+1 ; k < nbr_of_particles; k++) {

                double q1[nbr_of_dimensions];
                double q2[nbr_of_dimensions];
                for (int d = 0; d < nbr_of_dimensions; d++) {
                    q1[d] = qq(i,j,d);
                    q2[d] = qq(i,k,d);
                }
                double distance_sq = boundary_condition_dist_sq(q1, q2, ↩
                    cell_length);
                double dist = sqrt(distance_sq);
                int bin = get_bin(dist,min,max,d_r);
                bins2[bin] += 2;
            }
        }
    }
    double Nideal[k_bins];
    double factor =((double)(nbr_of_particles-1.0))/volume * 4.0*PI/3.0;
    for (int i = 0; i < k_bins; i++) {
        Nideal[i] = factor*(3.0*i*i-3.0*i+1.0)*d_r*d_r*d_r;
    }
```

```
274
275     /* Save data to file*/
276     file = fopen("histogram.dat","w");
277     for (int i = 0; i < k_bins; i ++) {
278         fprintf(file, "%e \t %i \t %i \t %e \n",d_r*(i-0.5), bins[i],bins2[i], ↩
                Nideal[i]);
279     }
280     fclose(file);
281     // TO THIS ISH TODO
282
283
284     free(energy_kin);       energy_kin = NULL;
285     free(energy);           energy = NULL;
286     free(disp_arr);         disp_arr = NULL;
287     free(virial);           virial = NULL;
288     free(temperature_avg);  temperature_avg = NULL;
289     free(pressure_avg);     pressure_avg = NULL;
290
291     return 0;
292 }
293
294 int get_bin(double val , double min , double max , double  d_r)
295 {
296     int bin = 0;
297     double current = min;
298     while (current <= val)
299     {
300         current += d_r;
301         bin++;
302     }
303     if (current > max)
304         return --bin;
305     return bin;
306 }
307
308 double boundary_condition_dist_sq(double u1[3], double u2[3], double L)
309 {
310     double d[3];
311     for (int i = 0; i < 3; i++) {
312         u1[i] /= L;
313         u2[i] /= L;
314
315         u1[i] -= floor(u1[i]);
316         d[i] = u1[i] - (u2[i] - floor(u2[i]));
317         d[i] -= (double)((int)floor(d[i]+0.5));
318     }
319
320     double sum = 0.0;
321     for (int i = 0; i < 3; i++)
322         sum += pow(d[i], 2);
323     return L*L * sum;
324
325 }
```

A.7 Task8/MD_main.c

```
1  /*
2   MD_main.c
3
4   Created by Anders Lindman on 2013-10-31.
5   */
6
7  #include <stdio.h>
8  #include <math.h>
9  #include <stdlib.h>
10 #include <time.h>
11 #include "initfcc.h"
12 #include "alpotential.h"
13 #include <complex.h>
14 #define nbr_of_particles 256
15 #define nbr_of_timesteps 1000
16 #define nbr_of_timesteps_eq 4000
17 #define nbr_of_dimensions 3
18
19 #define PI 3.141592653589
20 int get_bin(double , double , double , double );
21
22 double boundary_condition(double,double);
23
24 /* Main program */
25 int main()
26 {
27     srand(time(NULL));
28
29     /* Simulation parameters */
30     double m_AL; // Mass of atom
```

```
    double cell_length; // Side length of supercell
    double volume;
    double lattice_spacing; // Smallest length between atoms
    double initial_displacement;    // Initial displacement of the atoms from their
                                    // lattice positions
    double lattice_param;   // Lattice parameter, length of each side in the
                            // unit cell
    double timestep;
    double temperature_eq[] = { 1500.0+273.15, 700.0+273.15 };
    double pressure_eq = 101325e-11/1.602; // 1 atm in ASU
    double isothermal_compressibility = 1.0; //0.8645443196; // 1.385e-11 m^2/N = 1.385/1.602   ^3/eV

    FILE *file;


    /* Current displacement, velocities, and acceleratons */
    double q[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Displacements
    double v[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Velocities
    double f[nbr_of_particles][nbr_of_dimensions] = { 0 }; // Forces

    /* Allocate memory for large vectors */
    /* Simulate 3 dimensional data by placing iniitalizeing a 1-dimensional array*/
    #define qq(i,j,k) (disp_arr[nbr_of_particles*nbr_of_dimensions*i+nbr_of_dimensions*j+k])
    double* disp_arr = (double*)malloc(nbr_of_timesteps*nbr_of_particles*nbr_of_dimensions*sizeof(double));

    double* energy          = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* energy_kin      = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* virial          = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* temperature_avg = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* pressure_avg    = (double*) malloc(nbr_of_timesteps * sizeof(double));
    double* temperature     = (double*) malloc((2 * nbr_of_timesteps_eq + nbr_of_timesteps) * sizeof(double));
    double* pressure        = (double*) malloc((2 * nbr_of_timesteps_eq + nbr_of_timesteps) * sizeof(double));



    //TODO go over parameters again
    /* Initialize parameters*/
    initial_displacement    = 0.05;
    lattice_param           = 4.046; // For aluminium (  )
    lattice_spacing         = lattice_param/sqrt(2.0);
    timestep                = 0.01; // 0.1 Bad, 0.01 Seems decent
    m_AL                    = 0.0027964; // In ASU
    cell_length             = 4*lattice_param;  // Side of the supercell: The 256 atoms are
                                                // structured in a block of 4x4x4 unit cells
    volume                  = pow(cell_length, 3);

    // Initialize all displacements, for all times, as 0
    for (int i  = 0; i < nbr_of_timesteps; i++){
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                qq(i,j,k) = 0;
            }
        }
    }

    /* Put atoms on lattice */
    init_fcc(q, 4, lattice_param);


    /* Initial conditions */
    for (int i = 0; i < nbr_of_particles; i++){
        for (int j = 0; j < nbr_of_dimensions; j++){

            // Initial perturbation from equilibrium
            q[i][j] += lattice_spacing * initial_displacement
                * ((double)rand()/(double)RAND_MAX);

        }
    }


    get_forces_AL(f, q, cell_length, nbr_of_particles);

    /* Simulation */
    /* Equilibrium stage */

    double inst_temperature_eq;
```

```
    double inst_pressure_eq;
    double alpha_T = 1.0;
    double alpha_P = 1.0;
    double energy_kin_eq = get_kinetic_AL(v,nbr_of_dimensions,nbr_of_particles,m_AL);
    double virial_eq = get_virial_AL(q,cell_length,nbr_of_particles);

    temperature[0]  = instantaneous_temperature(energy_kin_eq, nbr_of_particles);
    pressure[0]     = instantaneous_pressure(virial_eq, temperature[0], nbr_of_particles, volume);

    for (int equil = 0; equil < 2; equil++) {
        for (int i = 1; i < nbr_of_timesteps_eq; i++)
        {
            /** Verlet algorithm **/
            /* Half step for velocity */
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
                }
            }

            /* Update displacement*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    q[j][k] += timestep * v[j][k];
                }
            }

            /* Forces */
            get_forces_AL(f,q,cell_length,nbr_of_particles);

            /* Final velocity*/
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] += timestep * 0.5* f[j][k]/m_AL;
                }
            }

            /* Calculate energy */
            // Kinetic energy
            energy_kin_eq = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles, m_AL);

            virial_eq = get_virial_AL(q, cell_length, nbr_of_particles);


            inst_temperature_eq = instantaneous_temperature(energy_kin_eq, nbr_of_particles);
            temperature[equil*(nbr_of_timesteps_eq-1) + i] = inst_temperature_eq;
            inst_pressure_eq = instantaneous_pressure(virial_eq, inst_temperature_eq,
                nbr_of_particles, volume);
            pressure[equil*(nbr_of_timesteps_eq-1) + i] = inst_pressure_eq;


            // Update alhpas
            alpha_T = 1.0 + 0.01*(temperature_eq[equil]-inst_temperature_eq)/inst_temperature_eq;
            alpha_P = 1.0 - 0.01*isothermal_compressibility*(pressure_eq - inst_pressure_eq);

            // DEBUG:alpha
            //printf("%.8f \t %.8f \n", alpha_T, alpha_P);

            // Scale velocities
            for (int j = 0; j < nbr_of_particles; j++){
                for (int k = 0; k < nbr_of_dimensions; k++){
                    v[j][k] *= sqrt(alpha_T);
                }
            }

            // Scale positions and volume
            cell_length *= pow(alpha_P, 1.0/3.0);
            volume = pow(cell_length, 3);
            for (int j = 0; j < nbr_of_particles; j++) {
                for (int k = 0; k < nbr_of_dimensions; k++) {
                    q[j][k] *= pow(alpha_P, 1.0/3.0);
                }
            }

        }
    }

    for (int i = 0; i < nbr_of_particles; i++){
        for (int j = 0; j < nbr_of_dimensions; j++){
            qq(0,i,j)=q[i][j];
        }
    }
```

```
    // Compute energies, temperature etc. at equilibrium
    energy[0] = get_energy_AL(q, cell_length, nbr_of_particles);
    virial[0] = get_virial_AL(q, cell_length, nbr_of_particles);
    energy_kin[0] = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles, m_AL)
        ;
    temperature_avg[0] = instantaneous_temperature(energy_kin[0],
         nbr_of_particles);
    pressure_avg[0] = instantaneous_pressure(virial[0], temperature_avg[0],
        nbr_of_particles, volume);

    /* Simulation after equilibrium*/
    for (int i = 1; i < nbr_of_timesteps; i++)
    {
        /** Verlet algorithm **/
        /* Half step for velocity */
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
            }
        }

        /* Update displacement*/
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                q[j][k] += timestep * v[j][k];
            }
        }

        /* Update Forces */
        get_forces_AL(f, q, cell_length, nbr_of_particles);

        /* Final velocity*/
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                v[j][k] += timestep * 0.5 * f[j][k]/m_AL;
            }
        }

        /* Calculate energy */
        // Potential energy
        energy[i] = get_energy_AL(q, cell_length, nbr_of_particles);
        // Kinetic energy
        energy_kin[i] = get_kinetic_AL(v, nbr_of_dimensions, nbr_of_particles,
             m_AL);

        virial[i] = get_virial_AL(q, cell_length, nbr_of_particles);

        // Temperature
        temperature_avg[i] = averaged_temperature(energy_kin, nbr_of_particles,
             i);
        temperature[2*(nbr_of_timesteps_eq-1) + i] = instantaneous_temperature(
             energy_kin[i],
            nbr_of_particles);


        // Pressure
        pressure_avg[i] = averaged_pressure(virial, energy_kin, volume, i);
        pressure[2*(nbr_of_timesteps_eq-1) + i] = instantaneous_pressure(virial[
             i],
            temperature[2*(nbr_of_timesteps_eq-1) + i],
            nbr_of_particles, volume);


        /* Save current displacements to array*/
        for (int j = 0; j < nbr_of_particles; j++){
            for (int k = 0; k < nbr_of_dimensions; k++){
                qq(i,j,k)=q[j][k];
            }
        }
    } // equilibration/simulation

    int n_x = 30;
    int n_y = 30;
    int n_z = 30;

    double factor = PI*2.0/cell_length;

    double qS[n_x][n_y][n_z][3];
    for (int i = 0; i < n_x; i++)
        for (int j = 0; j < n_y ; j++)
            for (int k = 0; k < n_z; k++){
                    qS[i][j][k][0]=i*factor;
                    qS[i][j][k][1]=j*factor;
                    qS[i][j][k][2]=k*factor;
                }

    double s[n_x][n_y][n_z];
    for (int i = 0; i < n_x; i++)
        for (int j = 0; j < n_y ; j++)
            for (int k = 0; k < n_z; k++)
```

```
            {
                if ( !((i==j) && (i==k) && (i==0))){
                    double complex sum = 0;
                    for (int r=0; r < nbr_of_particles; r++)
                    {
                        double complex expo=0;
                        for (int d = 0; d < nbr_of_dimensions; d++)
                        {
                            double ri = q[r][d];
                            ri=boundary_condition(ri,cell_length);
                            expo+= qS[i][j][k][d]*ri;
                        }
                        expo=expo*I;
                        sum+= cexp(expo);
                    }
                    sum = cabs(sum);
                    sum=sum*sum/nbr_of_particles;
                    s[i][j][k]=sum;
                }
            }

    double data[n_x*n_y*n_z];
    double dis[n_x*n_y*n_z];
    int iterator =0;
    for (int i = 0; i < n_x; i++)
        for (int j = 0; j < n_y ; j++)
            for (int k = 0; k < n_z; k++)
            {
                dis[iterator] =sqrt(1.0*i*i+1.0*j*j+1.0*k*k);
                data[iterator] = s[i][j][k];
                iterator++;
            }
    double max =0;
    double min = 1e10;
    for (int i = 0; i < n_x*n_y*n_z; i++ )
    {
        if (dis[i] > max)
            max = dis[i];
        if (dis[i] < min)
            min = dis[i];
    }

    int k_bins=200;
    double d_r = (max-min)/(1.0*k_bins);
    int bins[k_bins];
    for (int i = 0; i < n_x*n_y*n_z; i++)
    {
        int bin = get_bin(data[i],min,max,d_r);
        bins[bin]++;
    }

    file = fopen("data.dat","w");
    for (int i = 0; i < k_bins; i++)
    {
        fprintf(file, "%e \t %i \n", (double)(min+d_r*i*1.0), bins[i]);
    }

    fclose(file);
    /*
    file = fopen("data.dat","w");
    for (int i = 0; i < n_x*n_y*n_z; i ++)
    {
        fprintf(file, "%e \t %e \n",dis[i],data[i] );
    }
    fclose(file);*/

    free(energy_kin);       energy_kin = NULL;
    free(energy);           energy = NULL;
    free(disp_arr);         disp_arr = NULL;
    free(virial);           virial = NULL;
    free(temperature_avg);  temperature_avg = NULL;
    free(pressure_avg);     pressure_avg = NULL;

    return 0;
}

int get_bin(double val , double min , double max , double  d_r)
{
    int bin =0;
    double current=min;
    while (current <= val)
    {
        current += d_r;
        bin++;
    }
    return bin;
}

double boundary_condition(double u, double L)
{

```

```
    double f = fmod(u,L);
    if (f < 0)
        return -f;
    else
        return f;
}
```

```
/*
 alpotential.c
 Program that contains functions that calculate properties (potential energy, forces, etc.) of a set of Aluminum atoms using an embedded atom model (EAM) potential.
 Created by Anders Lindman on 2013-03-14.
 */


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

/*Parameters for the AL EAM potential */
#define PAIR_POTENTIAL_ROWS 18
const double pair_potential[90] = {2.0210, 2.2730, 2.4953, 2.7177, 2.9400, 3.1623, 3.3847, 3.6070, 3.8293, 4.0517, 4.2740, 4.4963, 4.7187, 4.9410, 5.1633, 5.3857, 5.6080, 6.0630, 2.0051, 0.7093, 0.2127, 0.0202, -0.0386, -0.0492, -0.0424, -0.0367, -0.0399, -0.0574, -0.0687, -0.0624, -0.0492, -0.0311, -0.0153, -0.0024, -0.0002, 0, -7.2241, -3.3383, -1.3713, -0.4753, -0.1171, 0.0069, 0.0374, 0.0122, -0.0524, -0.0818, -0.0090, 0.0499, 0.0735, 0.0788, 0.0686, 0.0339, -0.0012, 0, 9.3666, 6.0533, 2.7940, 1.2357, 0.3757, 0.1818, -0.0445, -0.0690, -0.2217, 0.0895, 0.2381, 0.0266, 0.0797, -0.0557, 0.0097, -0.1660, 0.0083, 0, -4.3827, -4.8865, -2.3363, -1.2893, -0.2907, -0.3393, -0.0367, -0.2290, 0.4667, 0.2227, -0.3170, 0.0796, -0.2031, 0.0980, -0.2634, 0.2612, -0.0102, 0};


#define ELECTRON_DENSITY_ROWS 15
const double electron_density[75] = {2.0210, 2.2730, 2.5055, 2.7380, 2.9705, 3.2030, 3.4355, 3.6680, 3.9005, 4.1330, 4.3655, 4.5980, 4.8305, 5.0630, 6.0630, 0.0824, 0.0918, 0.0883, 0.0775, 0.0647, 0.0512, 0.0392, 0.0291, 0.0186, 0.0082, 0.0044, 0.0034, 0.0027, 0.0025, 0.0000, 0.0707, 0.0071, -0.0344, -0.0533, -0.0578, -0.0560, -0.0465, -0.0428, -0.0486, -0.0318, -0.0069, -0.0035, -0.0016, -0.0008, 0, -0.1471, -0.1053, -0.0732, -0.0081, -0.0112, 0.0189, 0.0217, -0.0056, -0.0194, 0.0917, 0.0157, -0.0012, 0.0093, -0.0059, 0, 0.0554, 0.0460, 0.0932, -0.0044, 0.0432, 0.0040, -0.0392, -0.0198, 0.1593, -0.1089, -0.0242, 0.0150, -0.0218, 0.0042, 0};

#define EMBEDDING_ENERGY_ROWS 13
const double embedding_energy[65] = {0, 0.1000, 0.2000, 0.3000, 0.4000, 0.5000, 0.6000, 0.7000, 0.8000, 0.9000, 1.0000, 1.1000, 1.2000, 0, -1.1199, -1.4075, -1.7100, -1.9871, -2.2318, -2.4038, -2.5538, -2.6224, -2.6570, -2.6696, -2.6589, -2.6358, -18.4387, -5.3706, -2.3045, -3.1161, -2.6175, -2.0666, -1.6167, -1.1280, -0.4304, -0.2464, -0.0001, 0.1898, 0.2557, 86.5178, 44.1632, -13.5018, 5.3853, -0.3996, 5.9090, -1.4103, 6.2976, 0.6785, 1.1611, 1.3022, 0.5971, 0.0612, -141.1819, -192.2166, 62.9570, -19.2831, 21.0288, -24.3978, 25.6930, -18.7304, 1.6087, 0.4704, -2.3503, -1.7862, -1.7862};


#define k_b 0.00008617 // (eV)

/* Evaluates the spline in x. */

double splineEval(double x, const double *table,int m) {
    /* int m = mxGetM(spline), i, k;*/
    int i, k;

  /*double *table = mxGetPr(spline);*/
    double result;

    int k_lo = 0, k_hi = m;

    /* Find the index by bisection. */
    while (k_hi - k_lo > 1) {
        k = (k_hi + k_lo) >> 1;
        if (table[k] > x)
            k_hi = k;
        else
            k_lo = k;
    }

    /* Switch to local coord. */
    x -= table[k_lo];

    /* Horner's scheme */
    result = table[k_lo + 4*m];
    for (i = 3; i > 0; i--) {
        result *= x;
        result += table[k_lo + i*m];
```

```
    }

    return result;
}

/* Evaluates the derivative of the spline in x. */

double splineEvalDiff(double x, const double *table, int m) {
    /*int m = mxGetM(spline), i, k;
   double *table = mxGetPr(spline);
   */
  int i, k;
  double result;

    int k_lo = 0, k_hi = m;

    /* Find the index by bisection. */
    while (k_hi - k_lo > 1) {
        k = (k_hi + k_lo) >> 1;
        if (table[k] > x)
            k_hi = k;
        else
            k_lo = k;
    }

    /* Switch to local coord. */
    x -= table[k_lo];

    /* Horner's scheme */
    result = 3*table[k_lo + 4*m];
    for (i = 3; i > 1; i--) {
        result *= x;
        result += (i-1)*table[k_lo + i*m];
    }

    return result;
}

/* Returns the forces */
void get_forces_AL(double forces[][3], double positions[][3], double cell_length
    , int nbr_atoms)
{
  int i, j;
  double cell_length_inv, cell_length_sq;
  double rcut, rcut_sq;
  double densityi, dens, drho_dr, force;
  double dUpair_dr;
  double sxi, syi, szi, sxij, syij, szij, rij,  rij_sq;

  double *sx = malloc(nbr_atoms * sizeof (double));
  double *sy = malloc(nbr_atoms * sizeof (double));
  double *sz = malloc(nbr_atoms * sizeof (double));
  double *fx = malloc(nbr_atoms * sizeof (double));
  double *fy = malloc(nbr_atoms * sizeof (double));
  double *fz = malloc(nbr_atoms * sizeof (double));

  double *density = malloc(nbr_atoms * sizeof (double));
  double *dUembed_drho = malloc(nbr_atoms * sizeof (double));

  rcut = 6.06;
  rcut_sq = rcut * rcut;

  cell_length_inv = 1 / cell_length;
  cell_length_sq = cell_length * cell_length;

  for (i = 0; i < nbr_atoms; i++){
    sx[i] = positions[i][0] * cell_length_inv;
    sy[i] = positions[i][1] * cell_length_inv;
    sz[i] = positions[i][2] * cell_length_inv;
  }

  for (i = 0; i < nbr_atoms; i++){
    density[i] = 0;
    fx[i] = 0;
    fy[i] = 0;
    fz[i] = 0;
  }

  for (i = 0; i < nbr_atoms; i++) {
    /* Periodically translate coords of current particle to positive quadrants
        */
        sxi = sx[i] - floor(sx[i]);
        syi = sy[i] - floor(sy[i]);
        szi = sz[i] - floor(sz[i]);

    densityi = density[i];

        /* Loop over other atoms. */
        for (j = i + 1; j < nbr_atoms; j++) {
      /* Periodically translate atom j to positive quadrants and calculate
          distance to it. */
```

```
142             sxij = sxi - (sx[j] - floor(sx[j]));
143             syij = syi - (sy[j] - floor(sy[j]));
144             szij = szi - (sz[j] - floor(sz[j]));
145
146       /* Periodic boundary conditions. */
147             sxij = sxij - (int)floor(sxij + 0.5);
148             syij = syij - (int)floor(syij + 0.5);
149             szij = szij - (int)floor(szij + 0.5);
150
151       /* squared distance between atom i and j */
152             rij_sq = cell_length_sq * (sxij*sxij + syij*syij + szij*szij);
153
154       /* Add force and energy contribution if distance between atoms smaller ↩
              than rcut */
155             if (rij_sq < rcut_sq) {
156         rij = sqrt(rij_sq);
157         dens = splineEval(rij, electron_density, ELECTRON_DENSITY_ROWS);
158         densityi += dens;
159         density[j] += dens;
160       }
161     }
162     density[i] = densityi;
163   }
164
165   /* Loop over atoms to calculate derivative of embedding function
166    and embedding function. */
167     for (i = 0; i < nbr_atoms; i++) {
168         dUembed_drho[i] = splineEvalDiff(density[i], embedding_energy, ↩
                EMBEDDING_ENERGY_ROWS);
169     }
170
171   /* Compute forces on atoms. */
172     /* Loop over atoms again :-(. */
173
174   for (i = 0; i < nbr_atoms; i++) {
175     /* Periodically translate coords of current particle to positive quadrants ↩
           */
176         sxi = sx[i] - floor(sx[i]);
177         syi = sy[i] - floor(sy[i]);
178         szi = sz[i] - floor(sz[i]);
179
180     densityi = density[i];
181
182         /* Loop over other atoms. */
183         for (j = i + 1; j < nbr_atoms; j++) {
184       /* Periodically translate atom j to positive quadrants and calculate ↩
              distance to it. */
185             sxij = sxi - (sx[j] - floor(sx[j]));
186             syij = syi - (sy[j] - floor(sy[j]));
187             szij = szi - (sz[j] - floor(sz[j]));
188
189       /* Periodic boundary conditions. */
190             sxij = sxij - (int)floor(sxij + 0.5);
191             syij = syij - (int)floor(syij + 0.5);
192             szij = szij - (int)floor(szij + 0.5);
193
194       /* squared distance between atom i and j */
195             rij_sq = cell_length_sq * (sxij*sxij + syij*syij + szij*szij);
196
197       /* Add force and energy contribution if distance between atoms smaller ↩
              than rcut */
198             if (rij_sq < rcut_sq) {
199         rij = sqrt(rij_sq);
200         dUpair_dr = splineEvalDiff(rij, pair_potential, PAIR_POTENTIAL_ROWS);
201         drho_dr = splineEvalDiff(rij, electron_density, ELECTRON_DENSITY_ROWS);
202
203         /* Add force contribution from i-j interaction */
204                 force = -(dUpair_dr + (dUembed_drho[i] + dUembed_drho[j])*↩
                        drho_dr) / rij;
205                 fx[i] += force * sxij * cell_length;
206                 fy[i] += force * syij * cell_length;
207                 fz[i] += force * szij * cell_length;
208                 fx[j] -= force * sxij * cell_length;
209                 fy[j] -= force * syij * cell_length;
210                 fz[j] -= force * szij * cell_length;
211             }
212     }
213   }
214
215   for (i = 0; i < nbr_atoms; i++){
216     forces[i][0] = fx[i];
217     forces[i][1] = fy[i];
218     forces[i][2] = fz[i];
219   }
220
221   free(sx); free(sy); free(sz); sx = NULL; sy = NULL; sz = NULL;
222   free(fx); free(fy); free(fz); fx = NULL; fy = NULL; fz = NULL;
223   free(density); density = NULL;
224   free(dUembed_drho); dUembed_drho = NULL;
225
226 }
```

```
227
228 /* Returns the potential energy */
229 double get_energy_AL(double positions[][3], double cell_length, int nbr_atoms)
230 {
231   int i, j;
232   double cell_length_inv, cell_length_sq;
233   double rcut, rcut_sq;
234   double energy;
235   double densityi, dens;
236   double sxi, syi, szi, sxij, syij, szij, rij,  rij_sq;
237
238   double *sx = malloc(nbr_atoms * sizeof (double));
239   double *sy = malloc(nbr_atoms * sizeof (double));
240   double *sz = malloc(nbr_atoms * sizeof (double));
241
242   double *density = malloc(nbr_atoms * sizeof (double));
243
244   rcut = 6.06;
245   rcut_sq = rcut * rcut;
246
247   cell_length_inv = 1 / cell_length;
248   cell_length_sq = cell_length * cell_length;
249
250   for (i = 0; i < nbr_atoms; i++){
251     sx[i] = positions[i][0] * cell_length_inv;
252     sy[i] = positions[i][1] * cell_length_inv;
253     sz[i] = positions[i][2] * cell_length_inv;
254   }
255
256   for (i = 0; i < nbr_atoms; i++){
257     density[i] = 0;
258   }
259
260   energy = 0;
261
262   for (i = 0; i < nbr_atoms; i++) {
263     /* Periodically translate coords of current particle to positive quadrants ↩
          */
264         sxi = sx[i] - floor(sx[i]);
265         syi = sy[i] - floor(sy[i]);
266         szi = sz[i] - floor(sz[i]);
267
268     densityi = density[i];
269
270         /* Loop over other atoms. */
271         for (j = i + 1; j < nbr_atoms; j++) {
272       /* Periodically translate atom j to positive quadrants and calculate ↩
             distance to it. */
273             sxij = sxi - (sx[j] - floor(sx[j]));
274             syij = syi - (sy[j] - floor(sy[j]));
275             szij = szi - (sz[j] - floor(sz[j]));
276
277       /* Periodic boundary conditions. */
278             sxij = sxij - (int)floor(sxij + 0.5);
279             syij = syij - (int)floor(syij + 0.5);
280             szij = szij - (int)floor(szij + 0.5);
281
282       /* squared distance between atom i and j */
283             rij_sq = cell_length_sq * (sxij*sxij + syij*syij + szij*szij);
284
285       /* Add force and energy contribution if distance between atoms smaller ↩
            than rcut */
286             if (rij_sq < rcut_sq) {
287         rij = sqrt(rij_sq);
288         dens = splineEval(rij, electron_density, ELECTRON_DENSITY_ROWS);
289         densityi += dens;
290         density[j] += dens;
291
292         /* Add energy contribution from i-j interaction */
293         energy += splineEval(rij, pair_potential, PAIR_POTENTIAL_ROWS);
294
295       }
296     }
297     density[i] = densityi;
298   }
299
300   /* Loop over atoms to calculate derivative of embedding function
301    and embedding function. */
302     for (i = 0; i < nbr_atoms; i++) {
303         energy += splineEval(density[i], embedding_energy, EMBEDDING_ENERGY_ROWS↩
               );
304     }
305
306   free(sx); free(sy); free(sz); sx = NULL; sy = NULL; sz = NULL;
307   free(density); density = NULL;
308
309   return(energy);
310
311 }
312
313 /* Returns the virial */
```

```
double get_virial_AL(double positions[][3], double cell_length, int nbr_atoms)
{
  int i, j;
  double cell_length_inv, cell_length_sq;
  double rcut, rcut_sq;
  double virial;
  double densityi, dens, drho_dr, force;
  double dUpair_dr;
  double sxi, syi, szi, sxij, syij, szij, rij, rij_sq;

  double *sx = malloc(nbr_atoms * sizeof (double));
  double *sy = malloc(nbr_atoms * sizeof (double));
  double *sz = malloc(nbr_atoms * sizeof (double));

  double *density = malloc(nbr_atoms * sizeof (double));
  double *dUembed_drho = malloc(nbr_atoms * sizeof (double));

  rcut = 6.06;
  rcut_sq = rcut * rcut;

  cell_length_inv = 1 / cell_length;
  cell_length_sq = cell_length * cell_length;

  for (i = 0; i < nbr_atoms; i++){
    sx[i] = positions[i][0] * cell_length_inv;
    sy[i] = positions[i][1] * cell_length_inv;
    sz[i] = positions[i][2] * cell_length_inv;
  }

  for (i = 0; i < nbr_atoms; i++){
    density[i] = 0;
  }

  for (i = 0; i < nbr_atoms; i++) {
    /* Periodically translate coords of current particle to positive quadrants */
        sxi = sx[i] - floor(sx[i]);
        syi = sy[i] - floor(sy[i]);
        szi = sz[i] - floor(sz[i]);

    densityi = density[i];

        /* Loop over other atoms. */
        for (j = i + 1; j < nbr_atoms; j++) {
      /* Periodically translate atom j to positive quadrants and calculate
         distance to it. */
            sxij = sxi - (sx[j] - floor(sx[j]));
            syij = syi - (sy[j] - floor(sy[j]));
            szij = szi - (sz[j] - floor(sz[j]));

      /* Periodic boundary conditions. */
            sxij = sxij - (int)floor(sxij + 0.5);
            syij = syij - (int)floor(syij + 0.5);
            szij = szij - (int)floor(szij + 0.5);

      /* squared distance between atom i and j */
            rij_sq = cell_length_sq * (sxij*sxij + syij*syij + szij*szij);

      /* Add force and energy contribution if distance between atoms smaller
          than rcut */
            if (rij_sq < rcut_sq) {
        rij = sqrt(rij_sq);
        dens = splineEval(rij, electron_density, ELECTRON_DENSITY_ROWS);
        densityi += dens;
        density[j] += dens;
      }
    }
    density[i] = densityi;
  }

  /* Loop over atoms to calculate derivative of embedding function
   and embedding function. */
    for (i = 0; i < nbr_atoms; i++) {
        dUembed_drho[i] = splineEvalDiff(density[i], embedding_energy,
             EMBEDDING_ENERGY_ROWS);
    }

  /* Compute forces on atoms. */
    /* Loop over atoms again :-(. */

  virial = 0;

  for (i = 0; i < nbr_atoms; i++) {
    /* Periodically translate coords of current particle to positive quadrants */
        sxi = sx[i] - floor(sx[i]);
        syi = sy[i] - floor(sy[i]);
        szi = sz[i] - floor(sz[i]);

    densityi = density[i];

```

```
        /* Loop over other atoms. */
        for (j = i + 1; j < nbr_atoms; j++) {
      /* Periodically translate atom j to positive quadrants and calculate distance to it. */
            sxij = sxi - (sx[j] - floor(sx[j]));
            syij = syi - (sy[j] - floor(sy[j]));
            szij = szi - (sz[j] - floor(sz[j]));

      /* Periodic boundary conditions. */
            sxij = sxij - (int)floor(sxij + 0.5);
            syij = syij - (int)floor(syij + 0.5);
            szij = szij - (int)floor(szij + 0.5);

      /* squared distance between atom i and j */
            rij_sq = cell_length_sq * (sxij*sxij + syij*syij + szij*szij);

      /* Add force and energy contribution if distance between atoms smaller than rcut */
            if (rij_sq < rcut_sq) {
        rij = sqrt(rij_sq);
        dUpair_dr = splineEvalDiff(rij, pair_potential, PAIR_POTENTIAL_ROWS);
                drho_dr = splineEvalDiff(rij, electron_density, ELECTRON_DENSITY_ROWS);

        /* Add virial contribution from i-j interaction */
                force = -(dUpair_dr + (dUembed_drho[i] + dUembed_drho[j])*drho_dr) / rij;

        virial += force * rij_sq;
            }
    }
  }

  virial /= 3.0;

  free(sx); free(sy); free(sz); sx = NULL; sy = NULL; sz = NULL;
  free(density); density = NULL;
  free(dUembed_drho); dUembed_drho = NULL;

  return(virial);

}

double get_kinetic_AL(double velocities[][3], int nbr_of_dimensions, int nbr_atoms, double m_AL)
{
    double energy = 0;
    for (int j = 0; j < nbr_atoms; j++) {
        for (int k = 0; k < nbr_of_dimensions; k++) {
            energy += m_AL * pow(velocities[j][k], 2) / 2.0;
        }
    }
    return energy;
}


/* Calculation of instantaneous temperature, se 5.2 in molecular dynamics*/
double instantaneous_temperature(double kinetic_energy, int nbr_of_particles)
{
    double temperature = 0;
    temperature = 2.0/(k_b*nbr_of_particles*3) * kinetic_energy;
    return temperature;
}

/* Calculation of temperature based on averaged kinetic energy */
double averaged_temperature(double* kinetic_energy, int nbr_of_particles, int current_nbr_of_timesteps)
{
    double temperature = 0;
    double factor = 2.0/(3.0*k_b*nbr_of_particles*(current_nbr_of_timesteps+1.0));
    for (int i = 0; i < current_nbr_of_timesteps+1; i++)
    {
        temperature += kinetic_energy[i];
    }
    temperature*=factor;
    return temperature;
}


/* Calculation of instantaneous pressure, se 5.3 in molecular dynamics*/
double instantaneous_pressure(double virial, double temperature, int nbr_of_particles, double volume)
{
    //double pressure = 0;
    return (virial + temperature *k_b*nbr_of_particles) / volume;
}

/* Calculation of pressure based on averaged virial */
double averaged_pressure(double* virial, double* kinetic_energy, double volume, int current_nbr_of_timesteps)
```

```
{
    double pressure = 0;
    for (int i = 0; i < current_nbr_of_timesteps+1; i++)
    {
        pressure += (virial[i] + 2.0/3.0*kinetic_energy[i]);

    }
    pressure /= volume*(current_nbr_of_timesteps+1.0);
    return pressure;
}
```