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

H1b: MD simulation – dynamic properties

Andréas Sundström and Linnea Hesslow

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Task №	Points	Avail. points
Σ		

Introduction

The velocity Verlet algorithm is a semi-implicit and efficient method to simulate en ensemble of particles whose trajectories are governed by Newton's equation of motion. Accordingly, it is a suitable algorithm to study molecular dynamics and to determine statistical properties of a system. Here, we use the velocity Verlet algorithm to study a system of aluminum atoms in an fcc lattice. By scaling the positions, momenta and lattice parameter, we can equilibrate the temperature and pressure to prescribed values. We study the alumninum system at 500 ° C and 700 ° C, which correspond to the solid and liquid state respectively, and compute two dynamic quantities: mean square displacements and the velocity correlation function.

Task 1: potential energy

The theoretical lattice parameter for aluminim can be determined by calculating the minimum potential energy per unit cell in a lattice with zero initial momenta for all particles.

Figure 1 shows the potential energy as a function of the lattice parameter. We used a quadratic fit to find the minimum energy[1], and obtained $V_{\text{eq}} \approx 65.38\,\text{Å}^3$. This corresponds to the equilibrium lattice parameter $a_{\text{eq}} \approx 4.029\,\text{Å}$ at 0 K, which we took as the initial lattice parameter for the following tasks. We find that figure 1 looks similar to the figure 1 in the homework problem file, which is encouraging.

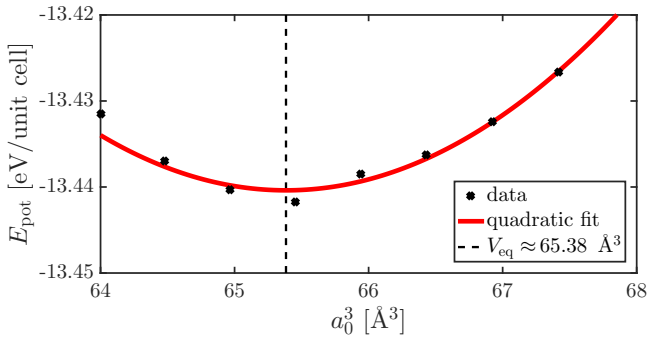

Figure 1: The potential energy per unit cell for aluminum as a function of the lattice parameter cubed.

Task 2: determine the time step

With the random noise, the temperature and the energy differ between runs, but are in the same order of magnitude. From figure 2, we determine that $dt = 5 \cdot 10^{-3}$ ps = 5 fs is a sufficient time step. This is in line with the lecture notes, where it is stated that a suitable timestep would normally be a few femtoseconds, or somewhat larger for heavy atoms. We note that the temperature in several cases is higher than desired value of 600-800 K from the problem sheet. The temperatures and energies up to one standard deviation are quantified in table 1.

Tasks 3 and 4: temperature and pressure equilibration

We set $\tau_P = \tau_T = 100dt$, where $dt = 5 \cdot 10^{-3}$ ps, and equilibrated the temperature and pressure by scaling the particle momenta and positions (and box size) respectively. Choosing a slower equilibration time did not affect the results qualitatively. Both temperature and pressure were equilibrated in the same Verlet loop, but for the higher temperature the the system was first melted by increasing the temperature to 900 °C. To

[1] We performed the quadratic fit in the volume V, which to a small error corresponds to a quadratic fit in the lattice parameter a, since $E \approx \alpha(V - V_0)^2 \approx \alpha a_0^4 (a - a_0)^2$ in a close vicinity of the minimum $a \approx a_0$

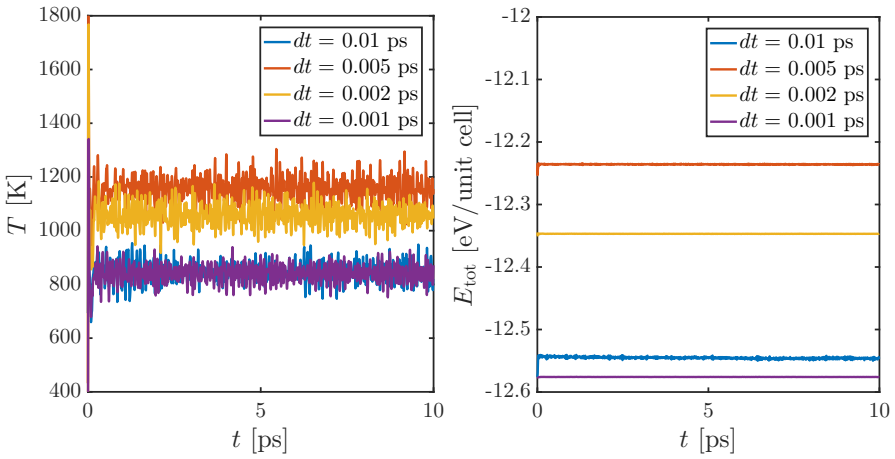

Figure 2: The temperature and kinetic energy per unit cell as a function of time for four different timesteps.

Table 1: Energies and temperatures with one standard deviation uncertainties for four different values of the time steps.

dt [ps]	T [K]	E_{tot} [eV/unit cell]
10^{-2}	$847 \pm 4.2\%$	$-12.55 \pm 1.2 \cdot 10^{-2}\%$
$5 \cdot 10^{-3}$	$1157 \pm 3.8\ \%$	$-12.24 \pm 3.6 \cdot 10^{-3}\%$
$2 \cdot 10^{-3}$	$1058 \pm 3.7\%$	$-12.35 \pm 6.6 \cdot 10^{-4}\%$
$1 \cdot 10^{-3}$	$841 \pm 3.7\%$	$-12.58 \pm 3.6 \cdot 10^{-4}\%$

determine the isothermal compressibility κ, the values of Young's modulus Y and shear modulus G were taken from Physics Handbook, table T 1.1. From F 1.15 in Physics Handbook, the bulk modulus can then calculated as

$$B = \frac{YG}{9G - 3Y} \qquad \kappa_{\text{Al}} = \frac{1}{B} \approx 6.6444 \cdot 10^5 \text{ bar}, \tag{1}$$

where $1\,\text{bar} = 6.2415 \cdot 10^{-7}\,\text{eV/Å}^3$ in atomic units. **However, we set $\kappa = 100\kappa_{\text{Al}}$ since the pressure equilibration happened on a much longer timescale than τ_P with $\kappa = \kappa_{\text{Al}}$. We have not yet figured out why this is.**

The results are shown in figure 3, where we overlay the instantaneous values of $\mathcal{T}$ and $\mathcal{P}$ with a moving average using 250 time steps. The desired temperatures and pressures were approximatelyh obtained in the equilibration process. Although the average pressure was slightly below zero, this is within the fluctuation error bars and is in line with the figure 2 in the homework problem document.

The equilibrium values of the lattice parameter were found to be

$$a_0 \approx 4.10\,\text{Å}, \quad T = 500\,^\circ\text{C}, \tag{2}$$

$$a_0 \approx 4.29\,\text{Å}, \quad T = 700\,^\circ\text{C}. \tag{3}$$

These value are larger than the zero-temperature constants, and it is reasonable that the higher 700 °C case corresponds to a larger lattice parameter at constant pressure.

Tasks 3-5: particle trajectories

Starting with the temperature- and pressure equilibrated systems from the previous section, we study the particle trajectories for both systems. Here, we decrease the timestep to $dt = 5 \cdot 10^{-4}$ ps and the simulation length to $t_{\text{end}} = 5$ ps to get better statistics. This was mostly motivated by increasing the resolution in tasks 6-7.

First, we note that the cumulative averages of the instantaneous temperatures and pressures stayed close to their inital values. This is shown in figure 4.

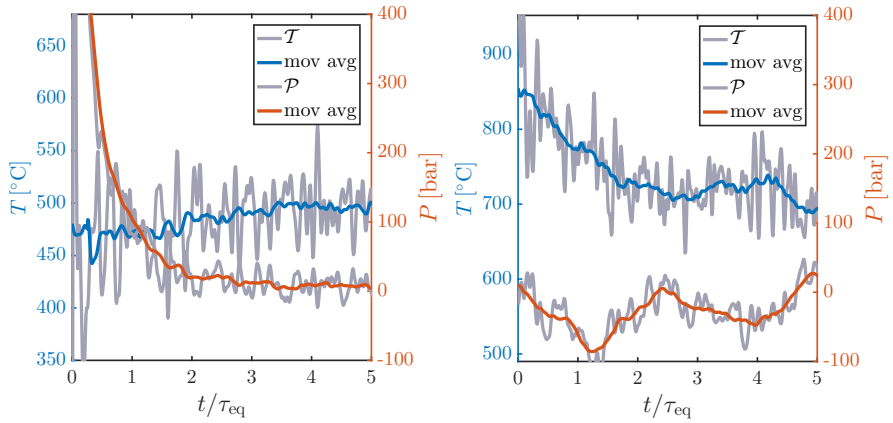

Figure 3: The instantaneous values of $\mathcal{T}$ and $\mathcal{P}$ overlayed with with a moving average using 100 time steps, which corresponds to $\Delta t = \tau_P/2$. Left panel: $T = 500\,^{\circ}\mathrm{C}$, right panel: $T = 700\,^{\circ}\mathrm{C}$.

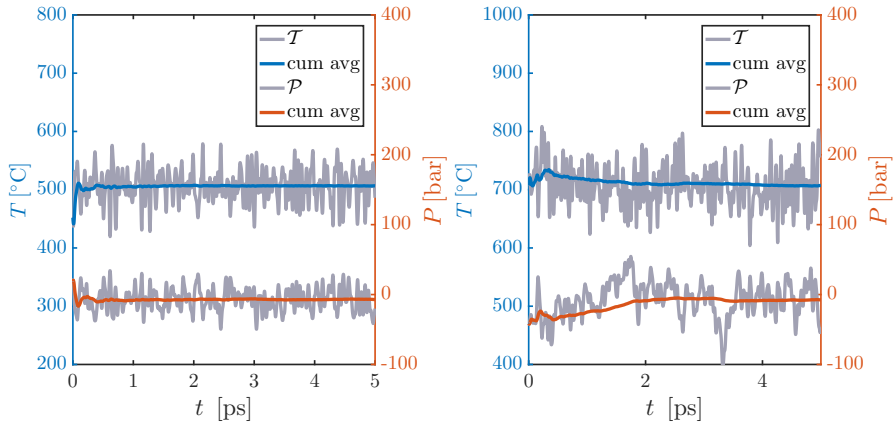

Figure 4: The instantaneous values, and the cumulative averages, of the temperature and the pressure in the production runs. Left panel: $T = 500\,^{\circ}\mathrm{C}$, right panel: $T = 700\,^{\circ}\mathrm{C}$

From equation (82) in MD lecture notes, the the means square displacement can be calculated as

$$\Delta_{\mathrm{MSD}}(t) = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt' \frac{1}{N_{\mathrm{atoms}}} \sum_{i=0}^{N_{\mathrm{atoms}}-1} \left[\mathbf{r}_i(t+t') - \mathbf{r}_i(t')\right]^2 \tag{4}$$

$$\Rightarrow$$

$$\Delta_{\mathrm{MSD}}(t_k) \approx \frac{1}{N_T - k} \frac{1}{N_{\mathrm{atoms}}} \sum_{j=0}^{N_T-k-1} \sum_{i=0}^{N_{\mathrm{atoms}}-1} \left[\mathbf{r}_i(t_{k+j}) - \mathbf{r}_i(t_j)\right]^2 \tag{5}$$

We now consider the particle trajectories. Figure 5 shows the trajectories of five individual particles along with the mean square displacement as determined in equation (5). We can clearly see that the particle trajectories are bounded in the left figure 5, while for the high-temperature case in the right panel, they increase as square root of time ($\Delta_{\mathrm{MSD}} \propto t$). Consequently, the former is in a solid state while the latter is in a liquid state.

The self-diffusion coefficient as determined by the average slope of the mean square displacement, was calculated to $D_s \approx 0.52\ \mathrm{Å}^2/\mathrm{ps}$.

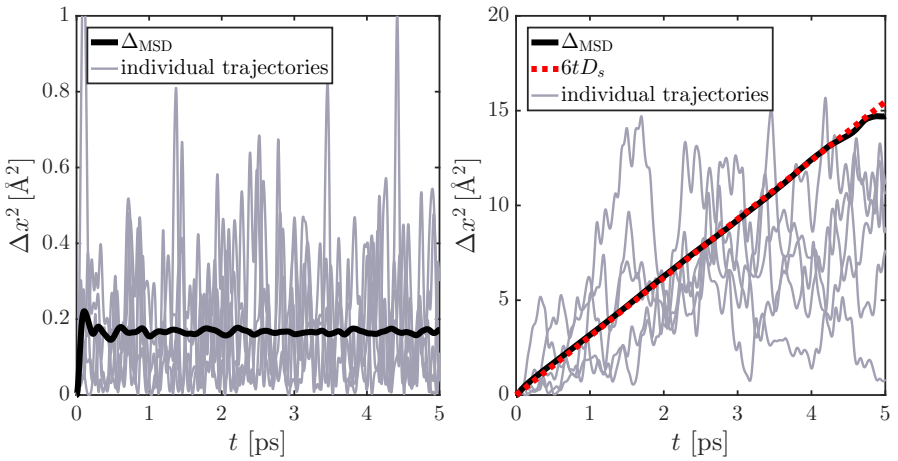

Figure 5: Five individual particle trajectories are shown in gray, overlaid with the mean square displacement in thick black line. In the left panel, $T = 500\,^{\circ}\mathrm{C}$, and the system is in a solid state. In the right panel, $T = 700\,^{\circ}\mathrm{C}$, the system is in a liquid state, where $\Delta_{\mathrm{MSD}} \approx 6tD_s$ (shown in dotted red).

Tasks 6-7: the velocity correlation

The average "power" content in avariable , $X(t')$, at some time, t, during some range of time, T, can be defined as

$$P_X(t,T) = \frac{1}{T}\int_{t-T/2}^{t+T/2} \mathrm{d}t'\ X^2(t'). \tag{6}$$

This quantity can (in physically relevant systems) also be defined for the process over all,

$$P_X = \lim_{T\to\infty} P_X(T) = \lim_{T\to\infty} \frac{1}{T}\left\langle \int_0^T \mathrm{d}t'\ X^2(t')\right\rangle. \tag{7}$$

At this stage, we can introduce a We have the Fourier transform

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, f(t)\mathrm{e}^{\mathrm{i}\omega t}, \tag{8}$$

Using these two functions, we can define a power spectrum

$$\begin{aligned}\hat{P}(\omega) &= \left\langle |\hat{\boldsymbol{v}}(\omega)|^2\right\rangle_{\mathrm{A}} = \left\langle \hat{\boldsymbol{v}}(\omega)\cdot\bar{\hat{\boldsymbol{v}}}(\omega)\right\rangle_{\mathrm{A}} \\ &= \left\langle \int_{-\infty}^{\infty} \mathrm{d}t\ \boldsymbol{v}(t)\mathrm{e}^{\mathrm{i}\omega t}\int_{-\infty}^{\infty}\mathrm{d}t'\ \boldsymbol{v}(t')\mathrm{e}^{-\mathrm{i}\omega t'}\right\rangle_{\mathrm{A}},\end{aligned} \tag{9}$$

where $\bar{\hat{\boldsymbol{v}}}$ denotes the complex conjugate of $\bar{\boldsymbol{v}}$. We can now change varaibles to $t = t' + \tau$ and note that the atom averages only falls on the velocities, which gives

$$\hat{P}(\omega) = \int_{-\infty}^{\infty}\mathrm{d}\tau\,\mathrm{e}^{\mathrm{i}\omega\tau}\int_{-\infty}^{\infty}\mathrm{d}t'\left\langle \boldsymbol{v}(t'+\tau)\cdot\boldsymbol{v}(t')\right\rangle_{\mathrm{A}}, \tag{10}$$

The self-diffusion coefficient as determined by the power spectral density at $f = 0$, was found to be $D_s = 0.49\,\text{Å}^2/\text{ps}$, which is close to the value obtained from the mean square displacement, as expected.

Concluding discussion

Using the velocity Verlet algorithm, we study a system of alumnim atoms at 500 ° C and 700 ° C, which correspond to the solid and liquid state respectively.

From both the mean square displacements and the velocity correlation function, the solid state is clearly distinguishable from the liquid state. The mean square displacement reaches a constant value in the solid state, whereas it grows linearly with time in the

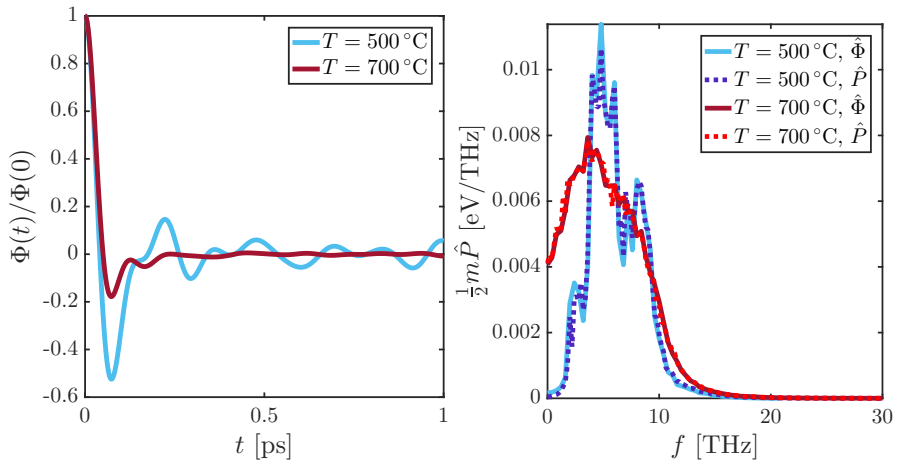

Figure 6: Left panel: The velocity correlation function, and (right panel) its spectrum, calculated both directly from the velocity correlation (solid line) and from the power spectrum of the particle velocity (dotted line). Blue lines show $T = 500\,^\circ$C and red lines $T = 700\,^\circ$C. The spectrum is multiplied by a factor of $\frac{1}{2}m_{\mathrm{Al}}$, in which case it can be interpreted as energy per frequency interval.

liquid state, which is characteristic of diffusion in a random walk process. Similarly, the spectrum of the velocity correlation function vanishes at zero frequency which means that the average velocity correlation is zero and hence there is no net movement of the particles; in contrast for the liquid state, the zero-frequency value of the spectrum is finite and proportional to the diffusion coefficient.

A Source Code

A.1 Main program task 1: `main_T1.c`

```c
/*
 main_T1.c Task 1 H1b
 */
#include <stdio.h>
#include <math.h>
#include <stdlib.h>

#include "initfcc.h"
#include "alpotential.h"

#define N_cells 4
#define N_lattice_params 25

/* Main program */
int main()
{
  int N_atoms = 4*N_cells*N_cells*N_cells;
  double a0;
  double a0_min = 4.0;
  double a0_max = 4.2;
  double da0 = (a0_max - a0_min)/N_lattice_params;

  double (*pos)[3] = malloc(sizeof(double[N_atoms][3]));
  double *energy = malloc(sizeof(double[N_lattice_params]));

  FILE *file_pointer;

  for (int i=0; i<N_lattice_params; i++){
    a0 = a0_min + i*da0;
    init_fcc(pos, N_cells, a0);
    // energy per unit cell
    energy[i] = get_energy_AL(pos, N_cells*a0, N_atoms )*4/N_atoms;
  }

  file_pointer = fopen("../data/lattice_energies.tsv", "w");
  for (int i=0; i<N_lattice_params; i++){
    a0 = a0_min + i*da0;
    fprintf(file_pointer, "%.8f \t %.8f \n", a0, energy[i]);
  }
  fclose(file_pointer);

  free(pos); pos = NULL;
  free(energy); energy = NULL;
  return 0;
}
```

A.2 Main program Task 2: `main_T2.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"
#include "funcs.h"

#define N_cells 4
#define AMU 1.0364e-4
#define kB 8.6173303e-5

/* Main program */
int main()
{

  int N_atoms = 4*N_cells*N_cells*N_cells;
  double m_Al = 27*AMU;

  double a_eq = 4.03;

  double noise_amplitude = 6.5e-2 * a_eq;
  double t_max=10;
  double dt = 1e-3;
```

```
  int N_timesteps = t_max/dt;
  double t, E_kin;

  double (*pos)[3] = malloc(sizeof(double[N_atoms][3]));
  double (*momentum)[3] = malloc(sizeof(double[N_atoms][3]));
  double (*forces)[3] = malloc(sizeof(double[N_atoms][3]));
  double *temperature = malloc(sizeof(double[N_timesteps]));
  double *E_tot = malloc(sizeof(double[N_timesteps]));

  FILE *file_pointer;


  /* ------------------------------ TASK 2 ----------------------------------*/

  init_fcc(pos, N_cells, a_eq); // initialize fcc lattice
  add_noise( N_atoms, 3, pos, noise_amplitude ); // adds random noise to pos
  set_zero( N_atoms, 3, momentum); // set momentum to 0
  get_forces_AL( forces, pos, a_eq*N_cells, N_atoms); //initial cond forces

  for (int i=0; i<N_timesteps; i++){
    /*
       The loop over the timesteps first takes a timestep according to the
       Verlet algorithm, then calculates the energies and temeperature.
    */
    timestep_Verlet (N_atoms, pos,  momentum, forces, m_Al, dt, a_eq*N_cells);

    E_kin    = get_kin_energy(N_atoms, momentum, m_Al );
    E_tot[i] = (E_kin + get_energy_AL(pos, a_eq*N_cells, N_atoms))*4/N_atoms;

    /* 3N*kB*T/2 = 1/(2m) * \sum_{i=1}^{N} p_i^2  = p_sq/(2m) */
    temperature[i] =  E_kin * 2/(3*N_atoms*kB);
  }

  /* Write tempertaure to file */
  char file_name[100];
  sprintf(file_name,"../data/temperature_dt-%0.0e_Task2.tsv", dt);
  file_pointer = fopen(file_name, "w");
  for (int i=0; i<N_timesteps; i++){
    t = i*dt; // time at step i
    fprintf(file_pointer, "%.4f \t %.8f \n", t, temperature[i]);
  }
  fclose(file_pointer);

  /* Write total energy to file */
  sprintf(file_name,"../data/total_energy_dt-%0.0e_Task2.tsv", dt);
  file_pointer = fopen(file_name, "w");
  for (int i=0; i<N_timesteps; i++){
    t = i*dt; // time at step i
    fprintf(file_pointer, "%.4f \t %.8f \n", t, E_tot[i]);
  }
  fclose(file_pointer);

  free(pos); pos = NULL;
  free(momentum); momentum = NULL;
  free(forces); forces = NULL;
  free(temperature); temperature = NULL;
  free(E_tot); E_tot = NULL;
  return 0;
}
```

A.3 Temperature and pressure equilibration for tasks 3-7: `main_T3.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"
#include "funcs.h"

#define N_cells 4
/* define constants in atomic units: eV,   , ps, K */
#define AMU 1.0364e-4
#define degC_to_K 273.15
#define bar 6.2415e-07
#define kB 8.61733e-5

```

```
/* Main program */
int main()
{
   char file_name[100];

   int N_atoms = 4*N_cells*N_cells*N_cells;
   double m_Al = 27*AMU;
   /*
     Values of Young's and shear modulus, Y and G resp., taken from
     Physics Handbook, table T 1.1. Bulk mudulus then calculated as
     B = Y*G / (9*G - 3*Y)   [F 1.15, Physics Handbook]
     kappa = 1/B
   */
   double kappa_Al = 100/(6.6444e+05 * bar); // STRANGE FACTOR 100 OFF !!!
   double a_eq = 4.03;
   double cell_length = a_eq*N_cells;
   double inv_volume = pow(N_cells*cell_length, -3);
   double noise_amplitude = 6.5e-2 * a_eq;

   double T_final_C= 500;
   int nRuns = 1; //2 if melt, 1 otherwise
   double T_melt_C = 900;

   double P_final_bar= 1;

  double T_eq;
  double P_eq  = P_final_bar*bar;
  double dt    = 5e-3;
  double tau_T = 100*dt;
  double tau_P = 100*dt;
  //double t_T_eq= 10*tau_T; //equlibration times
  double t_eq= 15*tau_P; //equlibration times
  int N_timesteps = t_eq/dt;

  double alpha_T, alpha_P,alpha_P_cube_root;
  double t, E_kin, virial;


  double (*pos)[3] = malloc(sizeof(double[N_atoms][3]));
  double (*momentum)[3] = malloc(sizeof(double[N_atoms][3]));
  double (*forces)[3] = malloc(sizeof(double[N_atoms][3]));
  double *temperature = malloc(sizeof(double[N_timesteps]));
  double *pressure = malloc(sizeof(double[N_timesteps]));


  FILE *file_pointer;

  /* ------------------------------ TASK 3 ----------------------------------*/


  init_fcc(pos, N_cells, a_eq); // initialize fcc lattice
  add_noise( N_atoms, 3, pos, noise_amplitude ); // adds random noise to pos
  set_zero( N_atoms, 3, momentum); // set momentum to 0
  get_forces_AL( forces, pos, cell_length, N_atoms); //initial cond forces

  /*
  for (int i=0; i<N_timesteps_T_eq; i++){
    //
       The loop over the timesteps first takes a timestep according to the
       Verlet algorithm, then calculates the energies and temeperature.
    //
    timestep_Verlet(N_atoms, pos,  momentum, forces, m_Al, dt, cell_length);

    E_kin  = get_kin_energy(N_atoms, momentum, m_Al );
    virial = get_virial_AL(pos, cell_length, N_atoms);

    // PV = NkT + virial
    pressure[i] = inv_volume * (1.5*E_kin + virial);
    // 3N*kB*T/2 = 1/(2m) * \sum_{i=1}^{N} p_i^2  = p_sq/(2m)
    temperature[i] =  E_kin * 1/(1.5*N_atoms*kB);


    alpha_T = 1 + 2*dt*(T_eq - temperature[i]) / (tau_T * temperature[i]);
    scale_mat(N_atoms, 3, momentum, sqrt(alpha_T));
    temperature[i]*=alpha_T;
  }
  */


    for (int irun=0; irun < nRuns; irun++){// last run: final, irun = 0
       if (irun == nRuns - 1){ // final run
          T_eq = T_final_C + degC_to_K;
       }else{
          T_eq = T_melt_C + degC_to_K;
       }
        for (int i=0; i<N_timesteps; i++){
      /*
         The loop over the timesteps first takes a timestep according to the
         Verlet algorithm, then calculates the energies and temeperature.
      */
      timestep_Verlet(N_atoms, pos,  momentum, forces, m_Al, dt, cell_length);
```

```
114
115
116         E_kin  = get_kin_energy(N_atoms, momentum, m_Al );
117         virial = get_virial_AL(pos, cell_length, N_atoms);
118
119         /* 3N*kB*T/2 = 1/(2m) * \sum_{i=1}^{N} p_i^2  = p_sq/(2m) */
120         temperature[i] =  E_kin * 1/(1.5*N_atoms*kB);
121         /* PV = NkT + virial */
122         pressure[i] = inv_volume * (1.5*E_kin + virial);
123
124         /* Equlibrate temperature by scaling momentum by a factor sqrt(alpha_T).
125             N.B. It is equally valid to scale the momentum instead of the velocity↩
                ,
126             since they only differ by a constant factor m.
127         */
128         alpha_T = 1 + 2*dt*(T_eq - temperature[i]) / (tau_T * temperature[i]);
129         scale_mat(N_atoms, 3, momentum, sqrt(alpha_T));
130
131         // Equlibrate pressure by scaling the posistions by a factor of alpha_P↩
               ^(1/3)
132
133         alpha_P = 1 - kappa_Al* dt*(P_eq - pressure[i])/tau_P;
134         alpha_P_cube_root = pow(alpha_P, 1.0/3.0);
135         scale_mat(N_atoms, 3, pos, alpha_P_cube_root);
136
137         cell_length*=alpha_P_cube_root;
138         inv_volume*=1/alpha_P;
139
140         temperature[i]*=alpha_T;
141         pressure[i]*=alpha_P;
142         }
143       }
144
145       printf("equilibrium a0 = %.4f A\n", cell_length/N_cells);
146
147     /* Write tempertaure to file */
148     sprintf(file_name,"../data/temp-%d_pres-%d_Task3.tsv",
149         (int) T_final_C, (int) P_final_bar);
150     file_pointer = fopen(file_name, "w");
151     for (int i=0; i<N_timesteps; i++){
152       t = i*dt; // time at step i
153       fprintf(file_pointer, "%.4f \t %.8f \t %.8f \n",
154           t, temperature[i],pressure[i]);
155     }
156     fclose(file_pointer);
157
158     /* Write phase space coordinates to file */
159     sprintf(file_name,"../data/phase-space_temp-%d_pres-%d.tsv",
160         (int) T_final_C, (int) P_final_bar);
161     file_pointer = fopen(file_name, "w");
162     for (int i=0; i<N_atoms; i++){
163       for (int j=0;j<3;j++){
164         fprintf(file_pointer, " %.16e \t", pos[i][j]);
165       }
166       for (int j=0;j<3;j++){
167         fprintf(file_pointer, " %.16e \t", momentum[i][j]);
168       }
169       fprintf(file_pointer,"\n");
170     }
171     fclose(file_pointer);
172
173     /* save equlibrated position and momentum as a binary file */
174     sprintf(file_name,"../data/INIDATA_temp-%d_pres-%d.bin",
175         (int) T_final_C, (int) P_final_bar);
176     file_pointer = fopen(file_name, "wb");
177     fwrite(pos, sizeof(double), 3*N_atoms, file_pointer);
178     fwrite(momentum, sizeof(double), 3*N_atoms, file_pointer);
179     fwrite(&cell_length, sizeof(double), 1, file_pointer);
180     fclose(file_pointer);
181
182
183     /*
184     printf("T=%0.2f\tP=%0.2e\n",
185        temperature[N_timesteps-1],pressure[N_timesteps-1]);
186     */
187
188     free(pos); pos = NULL;
189     free(momentum); momentum = NULL;
190     free(forces); forces = NULL;
191     free(temperature); temperature = NULL;
192     free(pressure); pressure = NULL;
193     //free(volume); volume = NULL;
194     return 0;
195 }
```

A.4 Production runs for tasks 3-7 : `main_Prod.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"
#include "funcs.h"

#define N_cells 4
/* define constants in atomic units: eV,   , ps, K */
#define AMU 1.0364e-4
#define degC_to_K 273.15
#define bar 6.2415e-07
#define kB 8.61733e-5

/* Main program */
int main()
{
  char file_name[100];

  int N_atoms = 4*N_cells*N_cells*N_cells;
  double m_Al = 27*AMU;
  /*
    Values of Young's and shear modulus, Y and G resp., taken from
    Physics Handbook, table T 1.1. Bulk mudulus then calculated as
    B = Y*G / (9*G - 3*Y)   [F 1.15, Physics Handbook]
    kappa = 1/B
  */
//  double kappa_Al = 100/(6.6444e+05 * bar); // STRANGE FACTOR 100 OFF !!!
  double cell_length = 0;
  double inv_volume;


  double T_eq_C   = 500;
  double P_eq_bar = 1;
//  double T_eq     = T_eq_C + degC_to_K;
//  double P_eq     = P_eq_bar*bar;
  double dt       = 5e-4; // higher res for spectral function
  double t_end    = 5;
//  double tau_T = 100*dt;
//  double tau_P = 100*dt;

  int N_timesteps = t_end/dt;

  int N_between_steps = 1;
  int N_save_timesteps = N_timesteps / N_between_steps; //for the displacements
  int N_save_atoms = 5;

//  double alpha_T, alpha_P,alpha_P_cube_root;
  double t, E_kin, virial;

  double (*pos)[3]      = malloc(sizeof(double[N_atoms][3]));
  double (*pos_0)[3]    = malloc(sizeof(double[N_atoms][3]));
  double (*momentum)[3] = malloc(sizeof(double[N_atoms][3]));
  double (*forces)[3]   = malloc(sizeof(double[N_atoms][3]));
  double (*displacements)[N_save_atoms] =
            malloc(sizeof(double[N_save_timesteps][N_save_atoms]));
  double (*pos_all)[N_atoms][3] =
            malloc(sizeof(double[N_save_timesteps][N_atoms][3]));
  double (*vel_all)[N_atoms][3] =
            malloc(sizeof(double[N_save_timesteps][N_atoms][3]));
  double *temperature   = malloc(sizeof(double[N_timesteps]));
  double *pressure      = malloc(sizeof(double[N_timesteps]));
  double *msd           = malloc(sizeof(double[N_save_timesteps]));
  double *vel_corr      = malloc(sizeof(double[N_save_timesteps]));
  double *pow_spec      = malloc(sizeof(double[N_save_timesteps]));
  double *freq            = malloc(sizeof(double[N_save_timesteps]));

  for (int i = 0; i<N_save_timesteps; i++){
    msd[i] = 0;
    pow_spec[i] = 0;
    vel_corr[i] = 0;
  }
  FILE *file_pointer;

  /* ------------------------------ TASK 3 ---------------------------------*/

  // read positions, momenta and cell_length
  sprintf(file_name,"../data/INIDATA_temp-%d_pres-%d.bin",
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "rb");
  fread(pos, sizeof(double), 3*N_atoms, file_pointer);
  fread(momentum, sizeof(double), 3*N_atoms, file_pointer);
```

```
  fread(&cell_length, sizeof(double), 1, file_pointer);
  fclose(file_pointer);

  for (int i=0; i<N_atoms; i++){
    for (int j=0; j<3; j++){
      pos_0[i][j]=pos[i][j];
    }
  }
  inv_volume = pow(N_cells*cell_length, -3);
  get_forces_AL( forces, pos, cell_length, N_atoms); //initial cond forces

  printf("Initialized. Starting with Verlet timestepping.\n");
  for (int i=0; i<N_timesteps; i++){
    /*
       The loop over the timesteps first takes a timestep according to the
       Verlet algorithm, then calculates the energies and temeperature.
    */
    timestep_Verlet(N_atoms, pos,  momentum, forces, m_Al, dt, cell_length);

    E_kin  = get_kin_energy(N_atoms, momentum, m_Al );
    virial = get_virial_AL(pos, cell_length, N_atoms);

    /* PV = NkT + virial */
    pressure[i] = inv_volume * (1.5*E_kin + virial);
    /* 3N*kB*T/2 = 1/(2m) * \sum_{i=1}^{N} p_i^2  = p_sq/(2m) */
    temperature[i] =  E_kin * 1/(1.5*N_atoms*kB);

    if (i % N_between_steps == 0){
         int k = i/N_between_steps; // number of saved timesteps so far
          get_displacements (N_save_atoms,  pos, pos_0, displacements[k]);
         copy_mat(N_atoms, 3, pos, pos_all[k]);

         copy_mat(N_atoms, 3, momentum, vel_all[k]);
         scale_mat(N_atoms, 3, vel_all[k], 1/m_Al);
     }
    if ((i*10) % N_timesteps == 0){
       printf("done %d0 %% of Verlet timestepping\n", (i*10)/N_timesteps);
    }
  }
  printf("calculating MSD\n");
  get_MSD(N_atoms, N_save_timesteps, pos_all, msd);

  printf("calculating velocity correlation\n");
  get_vel_corr(N_atoms, N_save_timesteps, vel_all, vel_corr);

  printf("calculating power spectrum\n");
  get_powerspectrum(N_atoms, N_save_timesteps, vel_all, pow_spec);
  fft_freq(freq, dt, N_save_timesteps);



  printf("writing to file\n");
  /* Write tempertaure to file */

  sprintf(file_name,"../data/temp-%d_pres-%d_Prod-test.tsv",
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "w");
  for (int i=0; i<N_timesteps; i++){
    t = i*dt; // time at step i
    fprintf(file_pointer, "%.4f \t %.8f \t %.8f \n",
        t, temperature[i],pressure[i]);
  }
  fclose(file_pointer);

  /* Write displacements to file */
  sprintf(file_name,"../data/temp-%d_pres-%d_displacements.tsv",
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "w");
  for (int i=0; i<N_save_timesteps; i++){
    t = i*dt*N_between_steps; // time at step i
    fprintf(file_pointer, "%.4f", t);
    for (int j=0; j<N_save_atoms; j++){
        fprintf(file_pointer, "\t %.8f", displacements[i][j]);
     }
     fprintf(file_pointer, "\n");
  }
  fclose(file_pointer);

   /* Write MSD to file */
  sprintf(file_name,"../data/temp-%d_pres-%d_dynamicProperties.tsv",
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "w");
  // write header
  fprintf(file_pointer, "%% t[ps] \t MSD[A^2] \t vel_corr [A/ps]^2 \n");
  for (int i=0; i<N_save_timesteps; i++){
     t = i*dt*N_between_steps; // time at step i
     fprintf(file_pointer, "%.4f \t %.8f \t %.8f \n", t, msd[i], vel_corr[i]);
  }
  fclose(file_pointer);

  sprintf(file_name,"../data/temp-%d_pres-%d_power-spectrum.tsv",
```

```
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "w");
  // write header
  fprintf(file_pointer, "%% f[1/ps] \t P[A/ps]^2 \n");
  for (int i=0; i<N_save_timesteps/2; i++){ // only print from f=0 to f_crit
     fprintf(file_pointer, "%.4f \t %.8f \n", freq[i], pow_spec[i]);
  }
  fclose(file_pointer);

  free(pos);           pos = NULL;
  free(pos_0);         pos_0 = NULL;
  free(momentum);      momentum = NULL;
  free(forces);        forces = NULL;
  free(temperature);   temperature = NULL;
  free(pressure);      pressure = NULL;
  free(displacements); displacements = NULL;
  free(pos_all); pos_all = NULL;
  free(vel_all); vel_all = NULL;
  free(msd); msd = NULL;
  free(vel_corr); vel_corr = NULL;
  free(pow_spec); pow_spec = NULL;
  free(freq); freq = NULL;
  return 0;
}
```

A.5 Production runs for tasks 3-7 : `main_Prod.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"
#include "funcs.h"

#define N_cells 4
/* define constants in atomic units: eV,   , ps, K */
#define AMU 1.0364e-4
#define degC_to_K 273.15
#define bar 6.2415e-07
#define kB 8.61733e-5

/* Main program */
int main()
{
  char file_name[100];

  int N_atoms = 4*N_cells*N_cells*N_cells;
  double m_Al = 27*AMU;
  /*
    Values of Young's and shear modulus, Y and G resp., taken from
    Physics Handbook, table T 1.1. Bulk mudulus then calculated as
    B = Y*G / (9*G - 3*Y)   [F 1.15, Physics Handbook]
    kappa = 1/B
  */
//  double kappa_Al = 100/(6.6444e+05 * bar); // STRANGE FACTOR 100 OFF !!!
  double cell_length = 0;
  double inv_volume;


  double T_eq_C   = 500;
  double P_eq_bar = 1;
//  double T_eq     = T_eq_C + degC_to_K;
//  double P_eq     = P_eq_bar*bar;
  double dt       = 5e-4; // higher res for spectral function
  double t_end    = 5;
//  double tau_T = 100*dt;
//  double tau_P = 100*dt;

  int N_timesteps = t_end/dt;

  int N_between_steps = 1;
  int N_save_timesteps = N_timesteps / N_between_steps; //for the displacements
  int N_save_atoms = 5;

//  double alpha_T, alpha_P,alpha_P_cube_root;
  double t, E_kin, virial;

  double (*pos)[3]      = malloc(sizeof(double[N_atoms][3]));
```

```
  double (*pos_0)[3]    = malloc(sizeof(double[N_atoms][3]));
  double (*momentum)[3] = malloc(sizeof(double[N_atoms][3]));
  double (*forces)[3]   = malloc(sizeof(double[N_atoms][3]));
  double (*displacements)[N_save_atoms] =
            malloc(sizeof(double[N_save_timesteps][N_save_atoms]));
  double (*pos_all)[N_atoms][3] =
            malloc(sizeof(double[N_save_timesteps][N_atoms][3]));
  double (*vel_all)[N_atoms][3] =
            malloc(sizeof(double[N_save_timesteps][N_atoms][3]));
  double *temperature   = malloc(sizeof(double[N_timesteps]));
  double *pressure      = malloc(sizeof(double[N_timesteps]));
  double *msd           = malloc(sizeof(double[N_save_timesteps]));
  double *vel_corr      = malloc(sizeof(double[N_save_timesteps]));
  double *pow_spec      = malloc(sizeof(double[N_save_timesteps]));
  double *freq            = malloc(sizeof(double[N_save_timesteps]));

  for (int i = 0; i<N_save_timesteps; i++){
    msd[i] = 0;
    pow_spec[i] = 0;
    vel_corr[i] = 0;
  }
  FILE *file_pointer;

  /* ----------------------------- TASK 3 ----------------------------------*/

  // read positions, momenta and cell_length
  sprintf(file_name,"../data/INIDATA_temp-%d_pres-%d.bin",
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "rb");
  fread(pos, sizeof(double), 3*N_atoms, file_pointer);
  fread(momentum, sizeof(double), 3*N_atoms, file_pointer);
  fread(&cell_length, sizeof(double), 1, file_pointer);
  fclose(file_pointer);

  for (int i=0; i<N_atoms; i++){
    for (int j=0; j<3; j++){
      pos_0[i][j]=pos[i][j];
    }
  }
  inv_volume = pow(N_cells*cell_length, -3);
  get_forces_AL( forces, pos, cell_length, N_atoms); //initial cond forces

  printf("Initialized. Starting with Verlet timestepping.\n");
  for (int i=0; i<N_timesteps; i++){
    /*
       The loop over the timesteps first takes a timestep according to the
       Verlet algorithm, then calculates the energies and temeperature.
    */
    timestep_Verlet(N_atoms, pos,  momentum, forces, m_Al, dt, cell_length);

    E_kin  = get_kin_energy(N_atoms, momentum, m_Al );
    virial = get_virial_AL(pos, cell_length, N_atoms);

    /* PV = NkT + virial */
    pressure[i] = inv_volume * (1.5*E_kin + virial);
    /* 3N*kB*T/2 = 1/(2m) * \sum_{i=1}^{N} p_i^2  = p_sq/(2m) */
    temperature[i] =  E_kin * 1/(1.5*N_atoms*kB);

    if (i % N_between_steps == 0){
         int k = i/N_between_steps; // number of saved timesteps so far
          get_displacements (N_save_atoms,  pos, pos_0, displacements[k]);
         copy_mat(N_atoms, 3, pos, pos_all[k]);

         copy_mat(N_atoms, 3, momentum, vel_all[k]);
         scale_mat(N_atoms, 3, vel_all[k], 1/m_Al);
     }
    if ((i*10) % N_timesteps == 0){
       printf("done %d0 %% of Verlet timestepping\n", (i*10)/N_timesteps);
    }
  }
  printf("calculating MSD\n");
  get_MSD(N_atoms, N_save_timesteps, pos_all, msd);

  printf("calculating velocity correlation\n");
  get_vel_corr(N_atoms, N_save_timesteps, vel_all, vel_corr);

  printf("calculating power spectrum\n");
  get_powerspectrum(N_atoms, N_save_timesteps, vel_all, pow_spec);
  fft_freq(freq, dt, N_save_timesteps);



  printf("writing to file\n");
  /* Write tempertaure to file */

  sprintf(file_name,"../data/temp-%d_pres-%d_Prod-test.tsv",
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "w");
  for (int i=0; i<N_timesteps; i++){
    t = i*dt; // time at step i
    fprintf(file_pointer, "%.4f \t %.8f \t %.8f \n",
```

```
        t, temperature[i],pressure[i]);
  }
  fclose(file_pointer);

  /* Write displacements to file */
  sprintf(file_name,"../data/temp-%d_pres-%d_displacements.tsv",
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "w");
  for (int i=0; i<N_save_timesteps; i++){
    t = i*dt*N_between_steps; // time at step i
    fprintf(file_pointer, "%.4f", t);
    for (int j=0; j<N_save_atoms; j++){
        fprintf(file_pointer, "\t %.8f", displacements[i][j]);
     }
     fprintf(file_pointer, "\n");
  }
  fclose(file_pointer);

   /* Write MSD to file */
  sprintf(file_name,"../data/temp-%d_pres-%d_dynamicProperties.tsv",
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "w");
  // write header
  fprintf(file_pointer, "%% t[ps] \t MSD[A^2] \t vel_corr [A/ps]^2 \n");
  for (int i=0; i<N_save_timesteps; i++){
     t = i*dt*N_between_steps; // time at step i
     fprintf(file_pointer, "%.4f \t %.8f \t %.8f \n", t, msd[i], vel_corr[i]);
  }
  fclose(file_pointer);

  sprintf(file_name,"../data/temp-%d_pres-%d_power-spectrum.tsv",
      (int) T_eq_C, (int) P_eq_bar);
  file_pointer = fopen(file_name, "w");
  // write header
  fprintf(file_pointer, "%% f[1/ps] \t P[A/ps]^2 \n");
  for (int i=0; i<N_save_timesteps/2; i++){ // only print from f=0 to f_crit
     fprintf(file_pointer, "%.4f \t %.8f \n", freq[i], pow_spec[i]);
  }
  fclose(file_pointer);

  free(pos);           pos = NULL;
  free(pos_0);         pos_0 = NULL;
  free(momentum);      momentum = NULL;
  free(forces);        forces = NULL;
  free(temperature);   temperature = NULL;
  free(pressure);      pressure = NULL;
  free(displacements); displacements = NULL;
  free(pos_all); pos_all = NULL;
  free(vel_all); vel_all = NULL;
  free(msd); msd = NULL;
  free(vel_corr); vel_corr = NULL;
  free(pow_spec); pow_spec = NULL;
  free(freq); freq = NULL;
  return 0;
}
```

A.6 Misc functions : `funcs.c`

```
#include "funcs.h"

void add_noise(int M, int N, double mat[M][N], double noise_amplitude )
{
  const  gsl_rng_type *T; /*  static  info  about  rngs */
  gsl_rng *q; /* rng  instance  */
  gsl_rng_env_setup (); /*  setup  the  rngs */
  T = gsl_rng_default; /*  specify  default  rng */
  q = gsl_rng_alloc(T); /*  allocate  default  rng */
  gsl_rng_set(q,time(NULL)); /*  Initialize  rng */

  for (int i=0; i<N; i++){
    for (int j=0; j<M; j++){
      // adds uniformly distributed random noise in range +-`noise_amplitude`
      mat[i][j] += noise_amplitude * (2*gsl_rng_uniform(q)-1);
    }
  }
  gsl_rng_free(q); /*  deallocate  rng */
}

void timestep_Verlet ( int N_atoms, double (*pos)[3],  double (*momentum)[3],
               double (*forces)[3], double m, double dt,
               double cell_length){
  for (int i = 0; i < N_atoms; i++) {
    for (int j = 0; j < 3; j++) {
      /* p(t+dt/2) */
      momentum[i][j] += dt * 0.5 * forces[i][j];
      /* q(t+dt) */
```

```
      pos[i][j] += dt * momentum[i][j] / m;
    }
  }
  /* F(t+dt) */
  get_forces_AL( forces, pos, cell_length, N_atoms);
  for (int i = 0; i < N_atoms; i++) {
    for (int j = 0; j < 3; j++) {
      /* p(t+dt/2) */
      momentum[i][j] += dt * 0.5 * forces[i][j];
    }
  }
}

double get_kin_energy ( int N_atoms,  double (*momentum)[3], double m ) {
  double p_sq=0; // momentum squared
  for (int i = 0; i < N_atoms; i++) {
    for (int j = 0; j < 3; j++) {
      p_sq += momentum[i][j] * momentum[i][j];
    }
  }
  return p_sq / (2*m);
}

void get_displacements ( int N_atoms,  double (*positions)[3],
             double (*initial_positions)[3], double disp[]) {
  for (int i = 0; i < N_atoms; i++) {
    for (int j = 0; j < 3; j++) {
      disp[i] += (positions[i][j] - initial_positions[i][j])
           *(positions[i][j] - initial_positions[i][j]);
    }
    disp[i] = sqrt(disp[i]);
  }
}


void get_MSD ( int N_atoms,  int N_times, double all_pos[N_times][N_atoms][3],
                  double MSD[N_times]) {
   /* all_pos = positions of all particles at all (saved) times */
   /* outer time index it starts at outer it = 1, since MSD[0] = 0*/
   for (int it = 1; it < N_times; it++) { //
      for (int jt = 0; jt < N_times-it; jt++) { // summed time index
         for (int kn = 0; kn < N_atoms; kn++) { // particle index
            for (int kd = 0; kd < 3; kd++) { // three dimensions
               MSD[it] += (all_pos[it+jt][kn][kd] - all_pos[jt][kn][kd])
                          *(all_pos[it+jt][kn][kd] - all_pos[jt][kn][kd]);
             }
          }
      }
      MSD[it] *= 1/( (double)N_atoms * (N_times-it));
   }
}

void get_vel_corr ( int N_atoms,  int N_times, double all_vel[N_times][N_atoms↩
    ][3],
                  double vel_corr[N_times]) {
   /* all_vel = velocity of all particles at all (saved) times */
   for (int it = 0; it < N_times; it++) { //
      for (int jt = 0; jt < N_times-it; jt++) { // summed time index
         for (int kn = 0; kn < N_atoms; kn++) { // particle index
            for (int kd = 0; kd < 3; kd++) { // three dimensions
               vel_corr[it] += (all_vel[it+jt][kn][kd] * all_vel[jt][kn][kd]);
             }
          }
      }
      vel_corr[it] *= 1/( (double)N_atoms * (N_times-it));
   }
}

void get_powerspectrum ( int N_atoms,  int N_times, double all_vel[N_times][↩
    N_atoms][3],
                  double pow_spec[N_times]) {
   /* all_vel = velocity of all particles at all (saved) times */
   double vel_component[N_times]; // "all_vel[:][i][j]"
   double pow_spec_component[N_times];
   double normalization_factor = 1/( (double)N_atoms * (N_times));
   for (int kn = 0; kn < N_atoms; kn++) { // particle index
    for (int kd = 0; kd < 3; kd++) { // three dimensions
         for (int it = 0; it < N_times; it++) { //
            vel_component[it] = all_vel[it][kn][kd];
          }
          powerspectrum(vel_component, pow_spec_component, N_times);
          for (int iw = 0; iw < N_times; iw++) { // for all frequencies
            pow_spec[iw] += pow_spec_component[iw];
          }
       }
   }
   for (int iw = 0; iw < N_times; iw++) { // for all frequencies
       pow_spec[iw] *= normalization_factor;
    }
}

```

```

void copy_mat (int M, int N, double mat_from[M][N], double mat_to[M][N]){
   /* Copies matrix `mat_from` to `mat_to` */
   for (int i = 0; i < M; i++) {
      for (int j = 0; j < N; j++) {
      mat_to[i][j] = mat_from[i][j];
      }
   }
}

void set_zero (int M, int N, double mat[M][N]){
  /* Sets the matrix `mat` to zero */
  for (int i = 0; i < M; i++) {
    for (int j = 0; j < N; j++) {
      mat[i][j] = 0;
    }
  }
}

void scale_mat (int M, int N, double mat[M][N], double alpha){
  /* Scales the matrix `mat` by factor `alpha` */
  for (int i = 0; i < M; i++) {
    for (int j = 0; j < N; j++) {
      mat[i][j] *= alpha;
    }
  }
}
```

B Auxiliary

B.1 Makefile

```

CC = gcc
CFLAGS = -O3 -Wall -Wno-unused-result

LIBS = -lm -lgsl -lgslcblas

HEADERS = initfcc.h alpotential.h funcs.h fft_func.h
OBJECTS = initfcc.o alpotential.o funcs.o fft_func.o


%.o: %.c $(HEADERS)
    $(CC) -c -o $@ $< $(CFLAGS)

all: Task1 Task2 Task3 main_Prod.c

Task1: $(OBJECTS) main_T1.c
    $(CC) -o $@ $^ $(CFLAGS) $(LIBS)

Task2: $(OBJECTS) main_T2.c
    $(CC) -o $@ $^ $(CFLAGS) $(LIBS)

Task3: $(OBJECTS) main_T3.c
    $(CC) -o $@ $^ $(CFLAGS) $(LIBS)

Prod: $(OBJECTS) main_Prod.c
    $(CC) -o $@ $^ $(CFLAGS) $(LIBS)

# $(PROGRAMS): $(OBJECTS) main_T1.c
#   $(CC) -o $@ $^ $(CFLAGS) $(LIBS)

clean:
    rm -f *.o
    touch *.c
```

C Matlab scripts

C.1 Analysis scripts for tasks 3-7: `Al_energies.m`

```
%% initial

tmp = matlab.desktop.editor.getActive; %% cd to current path
cd(fileparts(tmp.Filename));
set(0,'DefaultFigureWindowStyle','docked');
warning('off','MATLAB:handle_graphics:exceptions:SceneNode'); % interpreter ↩
     warning
```

```
GRAY = 0.7*[0.9 0.9 1];
AMU = 1.0364e-4;
m_Al = 27*AMU;
%% task 1: lattice energies
clc

energy_data = load('../data/lattice_energies.tsv');
a0 = energy_data(:,1);
v0 = a0.^3;

energy = energy_data(:,2);
figure(1);clf;
plot(v0,energy, 'xk');

start_v = 64;
end_v = 68;
indToInclude = (v0 > start_v) & (v0 < end_v);
p = polyfit(v0(indToInclude),energy(indToInclude),2);
hold on;

vvec = linspace(start_v, end_v);
plot(vvec, p(1)*vvec.^2 + p(2)*vvec + p(3), '-r');
xlim([64 68]);

v_min = -p(2)/(2*p(1));
a_min = v_min^(1/3);
omega_res = sqrt(2*p(1)*a_min^4/m_Al);
f_res = omega_res/(2*pi); % order of magnitude estimation of resonance frequency (?)

h1 = plot( v_min*[1 1], ax.YLim, '--k'); % plot vertical line at v_min

ax = gca; ax.YLim = [-13.45 -13.42];
ax.YTick = (-13.45:0.01:-13.42);
ylabel('$E_{\rm pot}$ [eV/unit cell]');
xlabel('$a_0^3$ [\AA$^3$]');
legend('data', 'quadratic fit', ['$V_{\rm eq} \approx \, $' num2str(round(v_min,2)) '\, \AA$^3$'], ...
    'location', 'southeast')
ax = gca; ax.Children = ax.Children(3:-1:1);
ImproveFigureCompPhys(gcf); h1.LineWidth = 2; setFigureSize(gcf, 300, 600);
saveas(gcf, '../figures/potential_energy.eps', 'epsc')
%% task 2: find a suitable timestep
clc;

dt=[1e-2,5e-3,2e-3,1e-3];
t_eq=0.5;

figure(1);clf;figure(2);clf;

for i=1:4
    T_data = load(sprintf('../data/temperature_dt-%0.0e_Task2.tsv',dt(i)));
    E_data = load(sprintf('../data/total_energy_dt-%0.0e_Task2.tsv',dt(i)));
    t = T_data(:,1);
    T = T_data(:,2);
    E = E_data(:,2);

    fprintf('dt = %0.0e\n',dt(i));

    T_avg=mean(T(t>t_eq));
    T_std=std(T(t>t_eq));
    fprintf('\tT = %0.2f +- %0.1f %%\n', T_avg, abs(T_std/T_avg)*100);

    E_avg=mean(E(t>t_eq));
    E_std=std(E(t>t_eq));
    fprintf('\tE = %0.2f +- %0.1e %%\n', E_avg, abs(E_std/E_avg)*100);

    figure(1)
    plot(t, T); hold on;

    figure(2)
    plot(t, E);hold on;
end
for ifig = 1:2
    figure(ifig);
    h = legend(strcat({'$dt = $ '}, num2str(round(dt',4)) , ' ps'));
    xlabel('$t$ [ps]');
    ax = gca;
    if ifig ==1
        ylabel('$T$ [K]')
        ax.YLim = [400 1800];
    else
        ylabel('$E_{\rm tot}$ [eV/unit cell]');
        ax.YTick = (-13:0.1:-10);
        ax.YLim = [-12.6 -12.0];
    end
    ImproveFigureCompPhys(gcf,'Linewidth', 2);setFigureSize(gcf, 400, 400);
end
saveas(1, '../figures/dt-scan-temperature.eps', 'epsc')
saveas(2, '../figures/dt-scan-energy.eps', 'epsc')
%% task 3: temperature and pressure equilibration,
```

```
% and task4: test production pressure and temperature

clc; clf;
temps = [500 700 500 700];
temperatures_str = num2str([500;700]);
FILENAMES = [strcat({'../data/temp-'}, temperatures_str, '_pres-1_Task3.tsv');
    strcat({'../data/temp-'}, temperatures_str, '_pres-1_Prod-test.tsv')];
bar = 6.2415e-07;
Kelvin_to_degC = -273.15;
t_eqs = [1 1 0.5 0.5]; % approximate equilibration time
N_average_points = 50;
dt = 5e-3;
tau_equilibration = 100*dt;

for iFile = 1:numel(FILENAMES)
    figure(iFile);clf;
    data = load(FILENAMES{iFile});

    t = data(:,1);
    T = data(:,2)+Kelvin_to_degC;
    P = data(:,3)/bar;

    t_eq=t_eqs(iFile);

    %fprintf('dt = %0.0e\n',dt(i));
    T_avg=mean(T(t>t_eq));
    T_std=std(T(t>t_eq));
    fprintf('\tT = %0.2f +- %0.1f K\n', T_avg, abs(T_std));

    P_avg=mean(P(t>t_eq));
    P_std=std(P(t>t_eq));
    fprintf('\tP = %0.2f +- %0.1f bar\n', P_avg, abs(P_std));

    yyaxis left

    if iFile <=2 % equlibration run, otherwise production
        plot(t./tau_equilibration,T, 'color', GRAY),hold on;
        plot(t./tau_equilibration, movmean(T,N_average_points),'-k')
    else
        plot(t,T, 'color', GRAY),hold on;
        plot(t, cumsum(T)./(1:length(t))','-k')
    end
    ylabel('$T \, [^\circ \rm C]$')

    if iFile <=2 % equlibration run, otherwise production
        ylim(temps(iFile)*(1+ 0.3*[-1,1.2]))
        yyaxis right
        plot(t./tau_equilibration,P),hold on;
        plot(t./tau_equilibration, movmean(P,N_average_points),'-k')
        legend('$\mathcal{T}$', 'mov avg','$\mathcal{P}$', 'mov avg');
        xlabel('$t/\tau_{\rm eq}$')
        xlim([0 5])
    else
        ylim(temps(iFile)+ 100*[-3,3])
        yyaxis right
        plot(t,P),hold on;
        plot(t, cumsum(P)./(1:length(t))','-k')
        legend('$\mathcal{T}$', 'cum avg','$\mathcal{P}$', 'cum avg');
        xlabel('$t$\, [ps]')
    end
    ylabel('$P \,[\rm bar]$')
    ylim([-100,400])
    ImproveFigureCompPhys(gcf, 'linewidth', 3, 'LineColor', {'MYORANGE', GRAY, '↩
        MYBLUE', GRAY}');
    setFigureSize(gcf, 400, 400);
end

saveas(1, '../figures/TP-eq-500.eps', 'epsc')
saveas(2, '../figures/TP-eq-700.eps', 'epsc')
saveas(3, '../figures/TP-prod-500.eps', 'epsc')
saveas(4, '../figures/TP-prod-700.eps', 'epsc')
%% determine displacements and MSD
temperatures_str = num2str([500;700]);
clc; clf;
figure(10); clf;
FILENAMES = strcat({'../data/temp-'}, temperatures_str, '_pres-1_displacements.↩
    tsv');
FILENAMES_Dyn = strcat({'../data/temp-'}, temperatures_str, '_pres-1↩
    _dynamicProperties.tsv');
FILENAMES_Pow = strcat({'../data/temp-'}, temperatures_str, '_pres-1_power-↩
    spectrum.tsv');
for iFile = 1:numel(FILENAMES)
    figure(iFile); clf;
    data = load(FILENAMES{iFile});
    t = data(:,1);
    dx = data(:,2:end);

    data = load(FILENAMES_Dyn{iFile});
    MSD = data(:,2);
    vel_corr = data(:,3);
    plot(t, MSD, 'k'); hold on;
```

```
    if iFile ==2 % liquid
        tStart = 1;
        D = MSD(t>tStart)./(6*t(t>tStart));
        selfDiffusionCoeff = mean(D); % in   ^2 /ps
        plot(t, 6*t*selfDiffusionCoeff, ':r');
    end

    plot(t, dx.^2, 'color', GRAY); hold on;

    xlabel('$t$ [ps]')
    ylabel('$\Delta x^2 \,[\rm \AA^2]$')
    if iFile ==1
        ylim([ 0 1.0]);
        leg = legend( '$\Delta_{\rm MSD}$', 'individual trajectories');
    else
        ylim([0 20]);
        leg = legend('$\Delta_{\rm MSD}$', '$6 t D_s$', 'individual trajectories');
    end

    leg.Location='northwest';
    ImproveFigureCompPhys(gcf, 'Linewidth', 2);
    ax = gca; [ax.Children(6:end).LineWidth] = deal(5);
    ax.Children = ax.Children([6:end 1:5]);
    setFigureSize(gcf, 400, 400);
end

% velocity correlation
figure(10);clf; figure(11);clf;
n_average_points = 1;%30;
for iFile = 1:numel(FILENAMES)
    data = load(FILENAMES_Dyn{iFile});
    t = data(:,1);
    vel_corr = data(:,3);

    data = load(FILENAMES_Pow{iFile});
    freq = data(:,1);
    pow_spec = data(:,2);

    figure(10);
    plot(t, vel_corr/vel_corr(1)); hold on;

    dt = t(2)-t(1);
    N_times = round(length(t)/2); % we have too bad statistics at later times.
    deltaf = 1/(N_times * dt);
    freqvec = 0:deltaf:(1/(2*dt));
    PhiHat = 2 * trapz(t(1:N_times), (vel_corr(1:N_times) * ones(size(freqvec)))
        .*     cos(2*pi*t(1:N_times) * freqvec ), 1); %dimension 1
    %PhiHat =  1/2 * 1/N_times * 2 * sum( (vel_corr(1:N_times) * ones(size(
        freqvec))) .* cos(2*pi*t(1:N_times) * freqvec ), 1); %dimension 1

    figure(11);
    plot(freqvec, m_Al/2*PhiHat); hold on;
    plot(freq, m_Al/2* pow_spec*t(end), ':'); hold on;
    if iFile ==2 % liquid
        tStart = 1;
        selfDiffusionCoeff_spectral = PhiHat(1)/6; % in   ^2 /ps
    end

end

disp([selfDiffusionCoeff selfDiffusionCoeff_spectral]);

figure(10)
xlim([0 1]);
leg = legend(strcat({'$T='}, num2str([500;700]), '\,^\circ $C'));
leg.Location='northeast';
xlabel('$t$ [ps]')
ylabel('$\Phi (t)/\Phi(0)$')
ImproveFigureCompPhys(gcf,'LineColor', {'MYRED', 'MYLIGHTBLUE'}');
setFigureSize(gcf, 400, 400);

figure(11)
leg = legend('$T= 500 \, ^\circ $C, $ \hat \Phi$' , '$T= 500 \, ^\circ $C, $\hat
    P$',...
    '$T= 700 \, ^\circ $C, $ \hat \Phi$', '$T= 700 \, ^\circ $C, $\hat P$');
xlim([0 30])
ylim([0 Inf])
xlabel('$f$ [THz]')
ylabel('$\frac{1}{2} m \hat P$ [eV/THz]')
setFigureSize(gcf, 400, 400);

ImproveFigureCompPhys(gcf,'LineColor', {'r', 'MYRED', 'GERIBLUE','MYLIGHTBLUE'
    }');


saveas(1, '../figures/MSD-500.eps', 'epsc')
saveas(2, '../figures/MSD-700.eps', 'epsc')
saveas(10, '../figures/Phi-t.eps', 'epsc')
saveas(11, '../figures/P-freq.eps', 'epsc')
```

C.2 Improve figure appearance: `ImproveFigureCompPhys.m`

```
function ImproveFigureCompPhys(varargin)
%ImproveFigureCompPhys Improves the figures of supplied handles
%  Input:
% - none (improve all figures) or handles to figures to improve
% - optional:
%       LineWidth  int
%       LineStyle  column vector cell, e.g. {'-','--'}',
%       LineColor  column vector cell, e.g. {'k',[0 1 1], 'MYBLUE'}'
%                          colors: MYBLUE,MYORANGE,MYGREEN,MYPURPLE, MYYELLOW,
%                          MYLIGHTBLUE, MYRED
%       Marker column vector cell, e.g. {'.', 'o', 'x'}'

% ImproveFigure was originally written by Adam Stahl, but has been heavily
% modified by Linnea Hesslow


%%% Handle inputs
% If no inputs or if the first argument is a string (a property rather than
% a handle), use all open figures
if nargin == 0 || ischar(varargin{1})
    %Get all open figures
    figHs = findobj('Type','figure');
    nFigs = length(figHs);
else
    % Check the supplied figure handles
    figHs = varargin{1};
    figHs = figHs(ishandle(figHs) == 1); %Keep only those handles that are ↩
        proper graphics handles
    nFigs = length(figHs);
end

% Define desired properties
titleSize = 24;
interpreter = 'latex';
lineWidth = 4;
axesWidth = 1.5;
labelSize = 22;
textSize = 20;
legTextSize = 18;
tickLabelSize = 18;
LineColor = {};
LineStyle = {};
Marker = {};

% define colors
co =  [ 0    0.4470    0.7410
    0.8500    0.3250    0.0980
    0.9290    0.6940    0.1250
    0.4940    0.1840    0.5560
    0.4660    0.6740    0.1880
    0.3010    0.7450    0.9330
    0.6350    0.0780    0.1840 ];
colors = struct('MYBLUE', co(1,:),...
    'MYORANGE', co(2,:),...
    'MYYELLOW', co(3,:),...
    'MYPURPLE', co(4,:),...
    'MYGREEN', co(5,:),...
    'MYLIGHTBLUE', co(6,:),...
    'MYRED',co(7,:),...
    'GERIBLUE', [0.3000    0.1500    0.7500],...
    'GERIRED', [1.0000    0.2500    0.1500],...
    'GERIYELLOW', [0.9000    0.7500    0.1000],...
    'LIGHTGREEN', [0.4    0.85    0.4],...
    'LINNEAGREEN', [7 184 4]/255);

% Loop through the supplied arguments and check for properties to set.
for i = 1:nargin
    if ischar(varargin{i})
        switch lower(varargin{i})   %Compare lower case strings
            case 'linewidth'
                lineWidth = varargin{i+1};
            case 'linestyle'
                LineStyle = varargin{i+1};
            case 'linecolor'
                LineColor = varargin{i+1};
                for iLineColor = 1:numel(LineColor)
                    if isfield(colors, LineColor{iLineColor})
                        LineColor{iLineColor} = colors.(LineColor{iLineColor});
                    end
                end
            case 'marker'
                Marker = varargin{i+1};
```

```
        end
    end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%% Improve the figure(s)

for iFig = 1:nFigs

    fig = figHs(iFig);

    lineObjects = findall(fig, 'Type', 'line');
    textObjects = findall(fig, 'Type', 'text');
    axesObjects = findall(fig, 'Type', 'axes');
    legObjects =  findall(fig, 'Type', 'legend');
    contourObjects = findall(fig,'Type','contour'); % not counted as lines

    %%% TEXT APPEARANCE: first set all to textSize and then change the ones
    %%% that need to be changed again

    %Change size of any text objects in the plot
    set(textObjects,'FontSize',textSize);
    set(legObjects,'FontSize',legTextSize);

    %%% FIX LINESTYLE, COLOR ETC. FOR EACH PLOT SEPARATELY
    for iAx =  1:numel(axesObjects)
        lineObjInAx = findall(axesObjects(iAx), 'Type', 'line');

        %set line style and color style (only works if all figs have some
        %number of line plots..)
        if ~isempty(LineStyle)
            set(lineObjInAx, {'LineStyle'}, LineStyle)
            set(contourObjects, {'LineStyle'}, LineStyle); %%%%%%
        end
        if ~isempty(LineColor)
            set(lineObjInAx, {'Color'}, LineColor)
            set(contourObjects, {'LineColor'}, LineColor); %%%%%%
        end
        if ~isempty(Marker)
            set(lineObjInAx, {'Marker'}, Marker)
            set(lineObjInAx, {'Markersize'}, num2cell(10+22*strcmp(Marker, '.'))↩
                )
        end

        %%% change font sizes.
        % Tick label size
        xLim = axesObjects(iAx).XLim;
        axesObjects(iAx).FontSize = tickLabelSize;
        axesObjects(iAx).XLim = xLim;
        %Change label size
        axesObjects(iAx).XLabel.FontSize = labelSize;
        axesObjects(iAx).YLabel.FontSize = labelSize;

        %Change title size
        axesObjects(iAx).Title.FontSize = titleSize;
    end

    %%% LINE APPEARANCE
    %Change line thicknesses
    set(lineObjects,'LineWidth',lineWidth);
    set(contourObjects, 'LineWidth', lineWidth);
    set(axesObjects, 'LineWidth',axesWidth)

    % set interpreter: latex or tex
    set(textObjects, 'interpreter', interpreter)
    set(legObjects, 'Interpreter', interpreter)
    set(axesObjects,'TickLabelInterpreter', interpreter);
end
end
```

C.3 Change size of figures: `setFigureSize.m`

```
function [ fig ] = setFigureSize( fig, H, W )
fig.Units = 'points';
fig.WindowStyle = 'normal'; % undock
fig.Position(3:4) = [W H];
end
```