

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

November 22, 2018

Task N ^o	Points	Avail. points
Σ		

Introduction

.... TODO... !!!!!!!!!!!!!!!!!!!!!!!

Task 1: potential energy

The theoretical lattice parameter for aluminum 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, and obtained $V_{\text{eq}} \approx 65.38 \text{ \AA}^3$. This corresponds to the equilibrium lattice parameter $a_{\text{eq}} \approx 4.029 \text{ \AA}$ at 0 K, which we took as the initial lattice parameter for the following tasks.

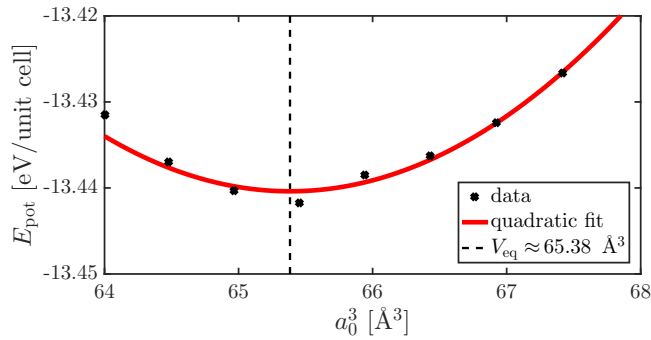


Figure 1: The potential energy per unit cell for aluminum as a function of the lattice parameter cubed.

We find that figure 1 looks similar to the figure 1 in the homework problem file.

Task 2: detmine the timestep

With the random noise, the temperature and the energy are differs between runs, but are in the same order of magnitude. From figure 2, we determine that $dt = 5 \cdot 10^{-3} \text{ ps} = 5 \text{ fs}$ is a sufficient time step. This is in line with the lecture notes, where it is stated that the a suitable timestep would normally be a few femtoseconds, or somewhat larger for heavy atoms.

We note that the temperature is higher than desired value of 600-800 K. The temperatures and energies up to one standard deviation are quantified in table 1.

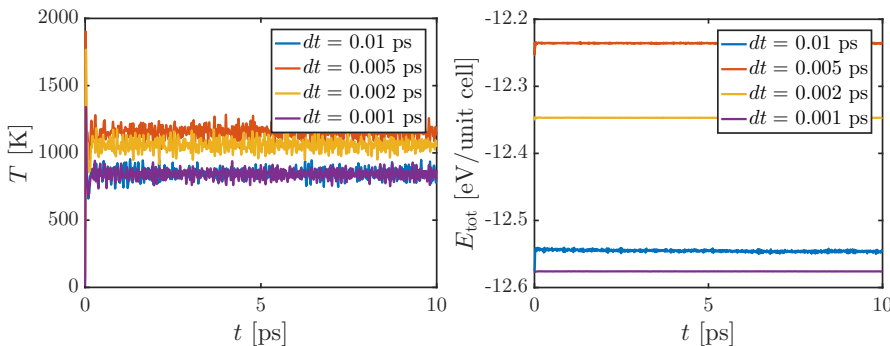


Figure 2: The temperature and kinetic energy per unit cell as a function of time for four different timesteps.

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}	$847 \pm 4.2\%$	$-12.55 \pm 1.2 \cdot 10^{-2}\%$
$5 \cdot 10^{-3}$	$1157 \pm 3.8\%$	$-12.24 \pm 3.6 \cdot 10^{-3}\%$
$2 \cdot 10^{-3}$	$1058 \pm 3.7\%$	$-12.35 \pm 6.6 \cdot 10^{-4}\%$
$1 \cdot 10^{-3}$	$841 \pm 3.7\%$	$-12.58 \pm 3.6 \cdot 10^{-4}\%$

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 system was first melted by increasing the temperature to 900 °C. To 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 be calculated as

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

where $1 \text{ bar} = 6.2415 \cdot 10^{-7} \text{ eV/\AA}^3$ 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 approximately 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.

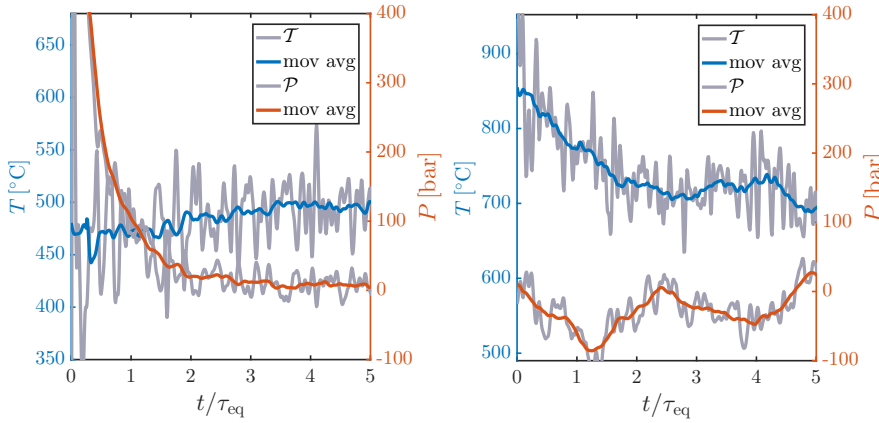


Figure 3: The instantaneous values of \mathcal{T} and \mathcal{P} overlaid with a moving average using 100 time steps, which corresponds to $\Delta t = \tau_P/2$. Left panel: $T = 500^\circ\text{C}$, right panel: $T = 700^\circ\text{C}$.

The equilibrium values of the lattice parameter were found to be

$$a_0 \approx 4.10 \text{ \AA}, \quad T = 500^\circ\text{C}, \quad (2)$$

$$a_0 \approx 4.29 \text{ \AA}, \quad T = 700^\circ\text{C}. \quad (3)$$

These values 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 initial values. This is shown in figure 4.

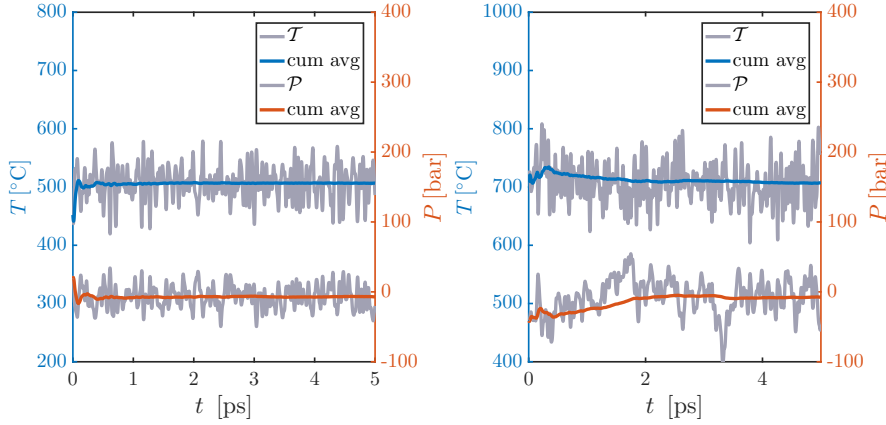


Figure 4: The instantaneous values, and the cumulative averages, of the temperature and the pressure in the production runs. Left panel: $T = 500$ °C, right panel: $T = 500$ °C

Task 5

Equation (82) in MD lecture notes:

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

\Rightarrow

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

To determine M, we used mean of ... for $t > \dots$

Task 7

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

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

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

$$P_X = \lim_{T \rightarrow \infty} P_X(T) = \lim_{T \rightarrow \infty} \frac{1}{T} \left\langle \int_0^T dt' X^2(t') \right\rangle. \quad (7)$$

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

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} dt f(t) e^{i\omega t}, \quad (8)$$

Using these two functions, we can define a power spectrum

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

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

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

Concluding discussion

!!!!!!!!!!!!!!!!!!!!!!!!!!!!1

A Source Code

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

A.1 Main program task 1: main_T1.c

```
1  /*
2   main_T1.c Task 1 H1b
3   */
4  #include <stdio.h>
5  #include <math.h>
6  #include <stdlib.h>
7
8  #include "initfcc.h"
9  #include "alpotential.h"
10
11 #define N_cells 4
12 #define N_lattice_params 25
13
14 /* Main program */
15 int main()
16 {
17     int N_atoms = 4*N_cells*N_cells*N_cells;
18     double a0;
19     double a0_min = 4.0;
20     double a0_max = 4.2;
21     double da0 = (a0_max - a0_min)/N_lattice_params;
22
23     double (*pos)[3] = malloc(sizeof(double[N_atoms][3]));
24     double *energy = malloc(sizeof(double[N_lattice_params]));
25
26     FILE *file_pointer;
27
28     for (int i=0; i<N_lattice_params; i++){
29         a0 = a0_min + i*da0;
30         init_fcc(pos, N_cells, a0);
31         // energy per unit cell
32         energy[i] = get_energy_AL(pos, N_cells*a0, N_atoms )*4/N_atoms;
33     }
34
35     file_pointer = fopen("../data/lattice_energies.tsv", "w");
36     for (int i=0; i<N_lattice_params; i++){
37         a0 = a0_min + i*da0;
38         fprintf(file_pointer, "%.8f \t %.8f \n", a0, energy[i]);
39     }
40     fclose(file_pointer);
41
42     free(pos); pos = NULL;
43     free(energy); energy = NULL;
44     return 0;
45 }
```

A.2 Main program Task 2: main_T2.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
12 #include "initfcc.h"
13 #include "alpotential.h"
14 #include "funcs.h"
15
16 #define N_cells 4
17 #define AMU 1.0364e-4
18 #define kB 8.6173303e-5
19
20 /* Main program */
21 int main()
22 {
23
24     int N_atoms = 4*N_cells*N_cells*N_cells;
```

```

25 double m_Al = 27*AMU;
26
27 double a_eq = 4.03;
28
29 double noise_amplitude = 6.5e-2 * a_eq;
30 double t_max=10;
31 double dt = 1e-3;
32 int N_timesteps = t_max/dt;
33 double t, E_kin;
34
35 double (*pos)[3] = malloc(sizeof(double[N_atoms][3]));
36 double (*momentum)[3] = malloc(sizeof(double[N_atoms][3]));
37 double (*forces)[3] = malloc(sizeof(double[N_atoms][3]));
38 double *temperature = malloc(sizeof(double[N_timesteps]));
39 double *E_tot = malloc(sizeof(double[N_timesteps]));
40
41 FILE *file_pointer;
42
43
44 /* ----- TASK 2 ----- */
45
46 init_fcc(pos, N_cells, a_eq); // initialize fcc lattice
47 add_noise( N_atoms, 3, pos, noise_amplitude ); // adds random noise to pos
48 set_zero( N_atoms, 3, momentum); // set momentum to 0
49 get_forces_AL( forces, pos, a_eq*N_cells, N_atoms); //initial cond forces
50
51 for (int i=0; i<N_timesteps; i++){
52     /*
53      * The loop over the timesteps first takes a timestep according to the
54      * Verlet algorithm, then calculates the energies and temeperature.
55      */
56     timestep_Verlet (N_atoms, pos, momentum, forces, m_Al, dt, a_eq*N_cells);
57
58     E_kin = get_kin_energy(N_atoms, momentum, m_Al );
59     E_tot[i] = (E_kin + get_energy_AL(pos, a_eq*N_cells, N_atoms))*4/N_atoms;
60
61     /*  $3NkB^*T/2 = 1/(2m) * \sum_{i=1}^N p_i^2 = p_{sq}/(2m)$  */
62     temperature[i] = E_kin * 2/(3*N_atoms*kB);
63 }
64
65 /* Write tempertaure to file */
66 char file_name[100];
67 sprintf(file_name, "../data/temperature_dt-%0.0e_Task2.tsv", dt);
68 file_pointer = fopen(file_name, "w");
69 for (int i=0; i<N_timesteps; i++){
70     t = i*dt; // time at step i
71     fprintf(file_pointer, "%.4f \t %.8f \n", t, temperature[i]);
72 }
73 fclose(file_pointer);
74
75 /* Write total energy to file */
76 sprintf(file_name, "../data/total_energy_dt-%0.0e_Task2.tsv", dt);
77 file_pointer = fopen(file_name, "w");
78 for (int i=0; i<N_timesteps; i++){
79     t = i*dt; // time at step i
80     fprintf(file_pointer, "%.4f \t %.8f \n", t, E_tot[i]);
81 }
82 fclose(file_pointer);
83
84 free(pos); pos = NULL;
85 free(momentum); momentum = NULL;
86 free(forces); forces = NULL;
87 free(temperature); temperature = NULL;
88 free(E_tot); E_tot = NULL;
89 return 0;
90 }

```

A.3 Temperature and pressure equilibration for tasks 3-7 : main_T3.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
12 #include "initfcc.h"
13 #include "alpotential.h"
14 #include "funcs.h"
15
16 #define N_cells 4
17 /* define constants in atomic units: eV, , ps, K */

```

```

18 #define AMU 1.0364e-4
19 #define degC_to_K 273.15
20 #define bar 6.2415e-07
21 #define kB 8.61733e-5
22
23 /* Main program */
24 int main()
25 {
26     char file_name[100];
27
28     int N_atoms = 4*N_cells*N_cells*N_cells;
29     double m_Al = 27*AMU;
30     /*
31      * Values of Young's and shear modulus, Y and G resp., taken from
32      * Physics Handbook, table T 1.1. Bulk modulus then calculated as
33      *  $B = Y * G / (9 * G - 3 * Y)$  [F 1.15, Physics Handbook]
34      *  $\kappa = 1/B$ 
35      */
36     double kappa_Al = 100/(6.6444e+05 * bar); // STRANGE FACTOR 100 OFF !!!
37     double a_eq = 4.03;
38     double cell_length = a_eq*N_cells;
39     double inv_volume = pow(N_cells*cell_length, -3);
40     double noise_amplitude = 6.5e-2 * a_eq;
41
42     double T_final_C= 500;
43     int nRuns = 1; //2 if melt, 1 otherwise
44     double T_melt_C = 900;
45
46     double P_final_bar= 1;
47
48     double T_eq;
49     double P_eq = P_final_bar*bar;
50     double dt = 5e-3;
51     double tau_T = 100*dt;
52     double tau_P = 100*dt;
53     //double t_Teq= 10*tau_T; //equilibration times
54     double t_eq= 15*tau_P; //equilibration times
55     int N_timesteps = t_eq/dt;
56
57     double alpha_T, alpha_P, alpha_P_cube_root;
58     double t, E_kin, virial;
59
60
61     double (*pos)[3] = malloc(sizeof(double[N_atoms][3]));
62     double (*momentum)[3] = malloc(sizeof(double[N_atoms][3]));
63     double (*forces)[3] = malloc(sizeof(double[N_atoms][3]));
64     double *temperature = malloc(sizeof(double[N_timesteps]));
65     double *pressure = malloc(sizeof(double[N_timesteps]));
66
67
68     FILE *file_pointer;
69
70     /* ----- TASK 3 ----- */
71
72
73     init_fcc(pos, N_cells, a_eq); // initialize fcc lattice
74     add_noise( N_atoms, 3, pos, noise_amplitude ); // adds random noise to pos
75     set_zero( N_atoms, 3, momentum); // set momentum to 0
76     get_forces_AL( forces, pos, cell_length, N_atoms); //initial cond forces
77
78     /*
79     for (int i=0; i<N_timesteps_Teq; i++){
80         //
81         The loop over the timesteps first takes a timestep according to the
82         Verlet algorithm, then calculates the energies and temeperature.
83         //
84         timestep_Verlet(N_atoms, pos, momentum, forces, m_Al, dt, cell_length);
85
86         E_kin = get_kin_energy(N_atoms, momentum, m_Al );
87         virial = get_virial_AL(pos, cell_length, N_atoms);
88
89         // PV = NkT + virial
90         pressure[i] = inv_volume * (1.5*E_kin + virial);
91         //  $3N * k_B * T / 2 = 1 / (2m) * \sum_{i=1}^N p_i^2 = p_{sq} / (2m)$ 
92         temperature[i] = E_kin * 1/(1.5*N_atoms*kB);
93
94
95         alpha_T = 1 + 2*dt*(T_eq - temperature[i]) / (tau_T * temperature[i]);
96         scale_mat(N_atoms, 3, momentum, sqrt(alpha_T));
97         temperature[i]*=alpha_T;
98     }
99     */
100
101
102     for (int irun=0; irun < nRuns; irun++){// last run: final, irun = 0
103         if (irun == nRuns - 1){ // final run
104             T_eq = T_final_C + degC_to_K;
105         }else{
106             T_eq = T_melt_C + degC_to_K;
107         }
108         for (int i=0; i<N_timesteps; i++){

```



```

109  /*
110     The loop over the timesteps first takes a timestep according to the
111     Verlet algorithm, then calculates the energies and temeperature.
112  */
113  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  /*  $3NkB T/2 = 1/(2m) * \sum_{i=1}^N p_i^2 = p_{sq}/(2m)$  */
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  /* Equilibrate 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  // Equilibrate pressure by scaling the posistions by a factor of alpha_P↔
132  //  $(1/3)$ 
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 equilibrated 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

```
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
12 #include "initfcc.h"
13 #include "alpotential.h"
14 #include "funcs.h"
15
16 #define N_cells 4
17 /* define constants in atomic units: eV, , ps, K */
18 #define AMU 1.0364e-4
19 #define degC_to_K 273.15
20 #define bar 6.2415e-07
21 #define kB 8.61733e-5
22
23 /* Main program */
24 int main()
25 {
26     char file_name[100];
27
28     int N_atoms = 4*N_cells*N_cells*N_cells;
29     double m_Al = 27*AMU;
30     /*
31      Values of Young's and shear modulus, Y and G resp., taken from
32      Physics Handbook, table T 1.1. Bulk modulus then calculated as
33      B = Y*G / (9*G - 3*Y) [F 1.15, Physics Handbook]
34      kappa = 1/B
35      */
36     // double kappa_Al = 100/(6.6444e+05 * bar); // STRANGE FACTOR 100 OFF !!!
37     double cell_length = 0;
38     double inv_volume;
39
40     double T_eq_C = 500;
41     double P_eq_bar = 1;
42     // double T_eq = T_eq_C + degC_to_K;
43     // double P_eq = P_eq_bar*bar;
44     double dt = 5e-4; // higher res for spectral function
45     double t_end = 5;
46     // double tau_T = 100*dt;
47     // double tau_P = 100*dt;
48
49     int N_timesteps = t_end/dt;
50
51     int N_between_steps = 1;
52     int N_save_timesteps = N_timesteps / N_between_steps; //for the displacements
53     int N_save_atoms = 5;
54
55     // double alpha_T, alpha_P, alpha_P_cube_root;
56     double t, E_kin, virial;
57
58     double (*pos)[3] = malloc(sizeof(double[N_atoms][3]));
59     double (*pos_0)[3] = malloc(sizeof(double[N_atoms][3]));
60     double (*momentum)[3] = malloc(sizeof(double[N_atoms][3]));
61     double (*forces)[3] = malloc(sizeof(double[N_atoms][3]));
62     double (*displacements)[N_save_atoms] =
63         malloc(sizeof(double[N_save_timesteps][N_save_atoms]));
64     double (*pos_all)[N_atoms][3] =
65         malloc(sizeof(double[N_save_timesteps][N_atoms][3]));
66     double (*vel_all)[N_atoms][3] =
67         malloc(sizeof(double[N_save_timesteps][N_atoms][3]));
68     double *temperature = malloc(sizeof(double[N_timesteps]));
69     double *pressure = malloc(sizeof(double[N_timesteps]));
70     double *msd = malloc(sizeof(double[N_save_timesteps]));
71     double *vel_corr = malloc(sizeof(double[N_save_timesteps]));
72     double *pow_spec = malloc(sizeof(double[N_save_timesteps]));
73     double *freq = malloc(sizeof(double[N_save_timesteps]));
74
75     for (int i = 0; i<N_save_timesteps; i++){
76         msd[i] = 0;
77         pow_spec[i] = 0;
78         vel_corr[i] = 0;
79     }
80     FILE *file_pointer;
81
82     /* ----- TASK 3 ----- */
83
84     // read positions, momenta and cell_length
85     sprintf(file_name, "../data/INIDATA_temp-%d_pres-%d.bin",
86
```

```

87     (int) T_eq_C, (int) P_eq_bar);
88     file_pointer = fopen(file_name, "rb");
89     fread(pos, sizeof(double), 3*N_atoms, file_pointer);
90     fread(momentum, sizeof(double), 3*N_atoms, file_pointer);
91     fread(&cell_length, sizeof(double), 1, file_pointer);
92     fclose(file_pointer);
93
94     for (int i=0; i<N_atoms; i++){
95         for (int j=0; j<3; j++){
96             pos_0[i][j]=pos[i][j];
97         }
98     }
99     inv_volume = pow(N_cells*cell_length, -3);
100     get_forces_AL( forces, pos, cell_length, N_atoms); //initial cond forces
101
102     printf("Initialized. Starting with Verlet timestepping.\n");
103     for (int i=0; i<N_timesteps; i++){
104         /*
105          * The loop over the timesteps first takes a timestep according to the
106          * Verlet algorithm, then calculates the energies and temeperature.
107          */
108         timestep_Verlet(N_atoms, pos, momentum, forces, m_Al, dt, cell_length);
109
110         E_kin = get_kin_energy(N_atoms, momentum, m_Al );
111         virial = get_virial_AL(pos, cell_length, N_atoms);
112
113         /* PV = NkT + virial */
114         pressure[i] = inv_volume * (1.5*E_kin + virial);
115         /* 3N*kB*T/2 = 1/(2m) * \sum_{i=1}^N p_i^2 = p_sq/(2m) */
116         temperature[i] = E_kin * 1/(1.5*N_atoms*kB);
117
118         if (i % N_between_steps == 0){
119             int k = i/N_between_steps; // number of saved timesteps so far
120             get_displacements (N_save_atoms, pos, pos_0, displacements[k]);
121             copy_mat(N_atoms, 3, pos, pos_all[k]);
122
123             copy_mat(N_atoms, 3, momentum, vel_all[k]);
124             scale_mat(N_atoms, 3, vel_all[k], 1/m_Al);
125         }
126         if ((i*10) % N_timesteps == 0){
127             printf("done %d %% of Verlet timestepping\n", (i*10)/N_timesteps);
128         }
129     }
130     printf("calculating MSD\n");
131     get_MSD(N_atoms, N_save_timesteps, pos_all, msd);
132
133     printf("calculating velocity correlation\n");
134     get_vel_corr(N_atoms, N_save_timesteps, vel_all, vel_corr);
135
136     printf("calculating power spectrum\n");
137     get_powerspectrum(N_atoms, N_save_timesteps, vel_all, pow_spec);
138     fft_freq(freq, dt, N_save_timesteps);
139
140
141
142     printf("writing to file\n");
143     /* Write tempertaure to file */
144
145     sprintf(file_name, "../data/temp-%d_pres-%d_Prod-test.tsv",
146             (int) T_eq_C, (int) P_eq_bar);
147     file_pointer = fopen(file_name, "w");
148     for (int i=0; i<N_timesteps; i++){
149         t = i*dt; // time at step i
150         fprintf(file_pointer, "%.4f \t %.8f \t %.8f \n",
151                 t, temperature[i], pressure[i]);
152     }
153     fclose(file_pointer);
154
155     /* Write displacements to file */
156     sprintf(file_name, "../data/temp-%d_pres-%d_displacements.tsv",
157             (int) T_eq_C, (int) P_eq_bar);
158     file_pointer = fopen(file_name, "w");
159     for (int i=0; i<N_save_timesteps; i++){
160         t = i*dt*N_between_steps; // time at step i
161         fprintf(file_pointer, "%.4f", t);
162         for (int j=0; j<N_save_atoms; j++){
163             fprintf(file_pointer, "\t %.8f", displacements[i][j]);
164         }
165         fprintf(file_pointer, "\n");
166     }
167     fclose(file_pointer);
168
169     /* Write MSD to file */
170     sprintf(file_name, "../data/temp-%d_pres-%d_dynamicProperties.tsv",
171             (int) T_eq_C, (int) P_eq_bar);
172     file_pointer = fopen(file_name, "w");
173     // write header
174     fprintf(file_pointer, "%\t [ps] \t MSD[A^2] \t vel_corr [A/ps]^2 \n");
175     for (int i=0; i<N_save_timesteps; i++){
176         t = i*dt*N_between_steps; // time at step i
177         fprintf(file_pointer, "%.4f \t %.8f \t %.8f \n", t, msd[i], vel_corr[i]);

```

```

178 }
179 fclose(file_pointer);
180
181 sprintf(file_name, "../data/temp-%d_pres-%d_power-spectrum.tsv",
182         (int) T_eq_C, (int) P_eq_bar);
183 file_pointer = fopen(file_name, "w");
184 // write header
185 fprintf(file_pointer, "%% f[1/ps] \t P[A/ps]^2 \n");
186 for (int i=0; i<N_save_timesteps/2; i++){ // only print from f=0 to f_crit
187     fprintf(file_pointer, "%.4f \t %.8f \n", freq[i], pow_spec[i]);
188 }
189 fclose(file_pointer);
190
191 free(pos);          pos = NULL;
192 free(pos_0);        pos_0 = NULL;
193 free(momentum);     momentum = NULL;
194 free(forces);        forces = NULL;
195 free(temperature);  temperature = NULL;
196 free(pressure);     pressure = NULL;
197 free(displacements); displacements = NULL;
198 free(pos_all); pos_all = NULL;
199 free(vel_all); vel_all = NULL;
200 free(msd); msd = NULL;
201 free(vel_corr); vel_corr = NULL;
202 free(pow_spec); pow_spec = NULL;
203 free(freq); freq = NULL;
204 return 0;
205 }

```

A.5 Production runs for tasks 3-7 : main_Prod.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
12 #include "initfcc.h"
13 #include "alpotential.h"
14 #include "funcs.h"
15
16 #define N_cells 4
17 /* define constants in atomic units: eV, , ps, K */
18 #define AMU 1.0364e-4
19 #define degC_to_K 273.15
20 #define bar 6.2415e-07
21 #define kB 8.61733e-5
22
23 /* Main program */
24 int main()
25 {
26     char file_name[100];
27
28     int N_atoms = 4*N_cells*N_cells*N_cells;
29     double m_Al = 27*AMU;
30     /*
31      Values of Young's and shear modulus, Y and G resp., taken from
32      Physics Handbook, table T 1.1. Bulk modulus then calculated as
33      B = Y*G / (9*G - 3*Y) [F 1.15, Physics Handbook]
34      kappa = 1/B
35      */
36     // double kappa_Al = 100/(6.6444e+05 * bar); // STRANGE FACTOR 100 OFF !!!
37     double cell_length = 0;
38     double inv_volume;
39
40     double T_eq_C = 500;
41     double P_eq_bar = 1;
42     // double T_eq = T_eq_C + degC_to_K;
43     // double P_eq = P_eq_bar*bar;
44     double dt = 5e-4; // higher res for spectral function
45     double t_end = 5;
46     // double tau_T = 100*dt;
47     // double tau_P = 100*dt;
48
49     int N_timesteps = t_end/dt;
50
51     int N_between_steps = 1;
52     int N_save_timesteps = N_timesteps / N_between_steps; //for the displacements
53     int N_save_atoms = 5;

```

```

56 // double alpha_T, alpha_P, alpha_P_cube_root;
57 double t, E_kin, virial;
58
59 double (*pos)[3] = malloc(sizeof(double[N_atoms][3]));
60 double (*pos_0)[3] = malloc(sizeof(double[N_atoms][3]));
61 double (*momentum)[3] = malloc(sizeof(double[N_atoms][3]));
62 double (*forces)[3] = malloc(sizeof(double[N_atoms][3]));
63 double (*displacements)[N_save_atoms] =
64     malloc(sizeof(double[N_save_timesteps][N_save_atoms]));
65 double (*pos_all)[N_atoms][3] =
66     malloc(sizeof(double[N_save_timesteps][N_atoms][3]));
67 double (*vel_all)[N_atoms][3] =
68     malloc(sizeof(double[N_save_timesteps][N_atoms][3]));
69 double *temperature = malloc(sizeof(double[N_timesteps]));
70 double *pressure = malloc(sizeof(double[N_timesteps]));
71 double *msd = malloc(sizeof(double[N_save_timesteps]));
72 double *vel_corr = malloc(sizeof(double[N_save_timesteps]));
73 double *pow_spec = malloc(sizeof(double[N_save_timesteps]));
74 double *freq = malloc(sizeof(double[N_save_timesteps]));
75
76 for (int i = 0; i < N_save_timesteps; i++){
77     msd[i] = 0;
78     pow_spec[i] = 0;
79     vel_corr[i] = 0;
80 }
81 FILE *file_pointer;
82
83 /* ----- TASK 3 ----- */
84
85 // read positions, momenta and cell_length
86 sprintf(file_name, "../data/INIDATA-temp-%d-pres-%d.bin",
87     (int) T_eq_C, (int) P_eq_bar);
88 file_pointer = fopen(file_name, "rb");
89 fread(pos, sizeof(double), 3*N_atoms, file_pointer);
90 fread(momentum, sizeof(double), 3*N_atoms, file_pointer);
91 fread(&cell_length, sizeof(double), 1, file_pointer);
92 fclose(file_pointer);
93
94 for (int i=0; i<N_atoms; i++){
95     for (int j=0; j<3; j++){
96         pos_0[i][j]=pos[i][j];
97     }
98 }
99 inv_volume = pow(N_cells*cell_length, -3);
100 get_forces_AL( forces, pos, cell_length, N_atoms); //initial cond forces
101
102 printf("Initialized. Starting with Verlet timestepping.\n");
103 for (int i=0; i<N_timesteps; i++){
104     /*
105      * The loop over the timesteps first takes a timestep according to the
106      * Verlet algorithm, then calculates the energies and temeperature.
107      */
108     timestep_Verlet(N_atoms, pos, momentum, forces, m_AL, dt, cell_length);
109
110     E_kin = get_kin_energy(N_atoms, momentum, m_AL);
111     virial = get_virial_AL(pos, cell_length, N_atoms);
112
113     /* PV = NkT + virial */
114     pressure[i] = inv_volume * (1.5*E_kin + virial);
115     /* 3N*kB*T/2 = 1/(2m) * \sum_{i=1}^N p_i^2 = p_sq/(2m) */
116     temperature[i] = E_kin * 1/(1.5*N_atoms*kB);
117
118     if (i % N_between_steps == 0){
119         int k = i/N_between_steps; // number of saved timesteps so far
120         get_displacements(N_save_atoms, pos, pos_0, displacements[k]);
121         copy_mat(N_atoms, 3, pos, pos_all[k]);
122
123         copy_mat(N_atoms, 3, momentum, vel_all[k]);
124         scale_mat(N_atoms, 3, vel_all[k], 1/m_AL);
125     }
126     if ((i*10) % N_timesteps == 0){
127         printf("done %d%% of Verlet timestepping\n", (i*10)/N_timesteps);
128     }
129 }
130 printf("calculating MSD\n");
131 get_MSD(N_atoms, N_save_timesteps, pos_all, msd);
132
133 printf("calculating velocity correlation\n");
134 get_vel_corr(N_atoms, N_save_timesteps, vel_all, vel_corr);
135
136 printf("calculating power spectrum\n");
137 get_powerspectrum(N_atoms, N_save_timesteps, vel_all, pow_spec);
138 fft_freq(freq, dt, N_save_timesteps);
139
140
141
142 printf("writing to file\n");
143 /* Write tempertaure to file */
144
145 sprintf(file_name, "../data/temp-%d-pres-%d-Prod-test.tsv",
146     (int) T_eq_C, (int) P_eq_bar);

```

```

147 file_pointer = fopen(file_name, "w");
148 for (int i=0; i<N_timesteps; i++){
149     t = i*dt; // time at step i
150     fprintf(file_pointer, "%.4f \t %.8f \t %.8f \n",
151         t, temperature[i], pressure[i]);
152 }
153 fclose(file_pointer);
154
155 /* Write displacements to file */
156 sprintf(file_name, "../data/temp-%d_pres-%d_displacements.tsv",
157     (int) T_eq_C, (int) P_eq_bar);
158 file_pointer = fopen(file_name, "w");
159 for (int i=0; i<N_save_timesteps; i++){
160     t = i*dt*N_between_steps; // time at step i
161     fprintf(file_pointer, "%.4f", t);
162     for (int j=0; j<N_save_atoms; j++){
163         fprintf(file_pointer, "\t %.8f", displacements[i][j]);
164     }
165     fprintf(file_pointer, "\n");
166 }
167 fclose(file_pointer);
168
169 /* Write MSD to file */
170 sprintf(file_name, "../data/temp-%d_pres-%d_dynamicProperties.tsv",
171     (int) T_eq_C, (int) P_eq_bar);
172 file_pointer = fopen(file_name, "w");
173 // write header
174 fprintf(file_pointer, "%s t[ps] \t MSD[A^2] \t vel_corr [A/ps]^2 \n");
175 for (int i=0; i<N_save_timesteps; i++){
176     t = i*dt*N_between_steps; // time at step i
177     fprintf(file_pointer, "%.4f \t %.8f \t %.8f \n", t, msd[i], vel_corr[i]);
178 }
179 fclose(file_pointer);
180
181 sprintf(file_name, "../data/temp-%d_pres-%d_power-spectrum.tsv",
182     (int) T_eq_C, (int) P_eq_bar);
183 file_pointer = fopen(file_name, "w");
184 // write header
185 fprintf(file_pointer, "%s f[1/ps] \t P[A/ps]^2 \n");
186 for (int i=0; i<N_save_timesteps/2; i++){ // only print from f=0 to f_crit
187     fprintf(file_pointer, "%.4f \t %.8f \n", freq[i], pow_spec[i]);
188 }
189 fclose(file_pointer);
190
191 free(pos);          pos = NULL;
192 free(pos_0);        pos_0 = NULL;
193 free(momentum);     momentum = NULL;
194 free(forces);        forces = NULL;
195 free(temperature);   temperature = NULL;
196 free(pressure);      pressure = NULL;
197 free(displacements); displacements = NULL;
198 free(pos_all);       pos_all = NULL;
199 free(vel_all);       vel_all = NULL;
200 free(msd);           msd = NULL;
201 free(vel_corr);      vel_corr = NULL;
202 free(pow_spec);      pow_spec = NULL;
203 free(freq);          freq = NULL;
204 return 0;
205 }

```

A.6 Misc functions : funcs.c

```

1 #include "funcs.h"
2
3 void add_noise(int M, int N, double mat[M][N], double noise_amplitude )
4 {
5     const gsl_rng_type *T; /* static info about rngs */
6     gsl_rng *q; /* rng instance */
7     gsl_rng_env_setup (); /* setup the rngs */
8     T = gsl_rng_default; /* specify default rng */
9     q = gsl_rng_alloc(T); /* allocate default rng */
10    gsl_rng_set(q, time(NULL)); /* Initialize rng */
11
12    for (int i=0; i<N; i++){
13        for (int j=0; j<M; j++){
14            // adds uniformly distributed random noise in range +/- noise_amplitude`
15            mat[i][j] += noise_amplitude * (2*gsl_rng_uniform(q)-1);
16        }
17    }
18    gsl_rng_free(q); /* deallocate rng */
19 }
20
21 void timestep_Verlet ( int N_atoms, double (*pos)[3], double (*momentum)[3],
22     double (*forces)[3], double m, double dt,
23     double cell_length){
24     for (int i = 0; i < N_atoms; i++) {

```

```

25     for (int j = 0; j < 3; j++) {
26         /* p(t+dt/2) */
27         momentum[i][j] += dt * 0.5 * forces[i][j];
28         /* q(t+dt) */
29         pos[i][j] += dt * momentum[i][j] / m;
30     }
31 }
32 /* F(t+dt) */
33 get_forces_AL( forces, pos, cell_length, N_atoms);
34 for (int i = 0; i < N_atoms; i++) {
35     for (int j = 0; j < 3; j++) {
36         /* p(t+dt/2) */
37         momentum[i][j] += dt * 0.5 * forces[i][j];
38     }
39 }
40 }
41
42 double get_kin_energy ( int N_atoms, double (*momentum)[3], double m ) {
43     double p_sq=0; // momentum squared
44     for (int i = 0; i < N_atoms; i++) {
45         for (int j = 0; j < 3; j++) {
46             p_sq += momentum[i][j] * momentum[i][j];
47         }
48     }
49     return p_sq / (2*m);
50 }
51
52 void get_displacements ( int N_atoms, double (*positions)[3],
53                         double (*initial_positions)[3], double disp[]) {
54     for (int i = 0; i < N_atoms; i++) {
55         for (int j = 0; j < 3; j++) {
56             disp[i] += (positions[i][j] - initial_positions[i][j])
57                       *(positions[i][j] - initial_positions[i][j]);
58         }
59         disp[i] = sqrt(disp[i]);
60     }
61 }
62
63 void get_MSD ( int N_atoms, int N_times, double all_pos[N_times][N_atoms][3],
64              double MSD[N_times]) {
65     /* all_pos = positions of all particles at all (saved) times */
66     /* outer time index it starts at outer it = 1, since MSD[0] = 0 */
67     for (int it = 1; it < N_times; it++) { //
68         for (int jt = 0; jt < N_times-it; jt++) { // summed time index
69             for (int kn = 0; kn < N_atoms; kn++) { // particle index
70                 for (int kd = 0; kd < 3; kd++) { // three dimensions
71                     MSD[it] += (all_pos[it+jt][kn][kd] - all_pos[jt][kn][kd])
72                               *(all_pos[it+jt][kn][kd] - all_pos[jt][kn][kd]);
73                 }
74             }
75         }
76         MSD[it] *= 1/( (double)N_atoms * (N_times-it));
77     }
78 }
79
80 void get_vel_corr ( int N_atoms, int N_times, double all_vel[N_times][N_atoms]←
81                   ][3],
82                   double vel_corr[N_times]) {
83     /* all_vel = velocity of all particles at all (saved) times */
84     for (int it = 0; it < N_times; it++) { //
85         for (int jt = 0; jt < N_times-it; jt++) { // summed time index
86             for (int kn = 0; kn < N_atoms; kn++) { // particle index
87                 for (int kd = 0; kd < 3; kd++) { // three dimensions
88                     vel_corr[it] += (all_vel[it+jt][kn][kd] * all_vel[jt][kn][kd]);
89                 }
90             }
91         }
92         vel_corr[it] *= 1/( (double)N_atoms * (N_times-it));
93     }
94 }
95
96 void get_powerspectrum ( int N_atoms, int N_times, double all_vel[N_times][←
97                       N_atoms][3],
98                       double pow_spec[N_times]) {
99     /* all_vel = velocity of all particles at all (saved) times */
100    double vel_component[N_times]; // "all_vel[:,i][j]"
101    double pow_spec_component[N_times];
102    double normalization_factor = 1/( (double)N_atoms * (N_times));
103    for (int kn = 0; kn < N_atoms; kn++) { // particle index
104        for (int kd = 0; kd < 3; kd++) { // three dimensions
105            for (int it = 0; it < N_times; it++) { //
106                vel_component[it] = all_vel[it][kn][kd];
107            }
108            powerspectrum(vel_component, pow_spec_component, N_times);
109            for (int iw = 0; iw < N_times; iw++) { // for all frequencies
110                pow_spec[iw] += pow_spec_component[iw];
111            }
112        }
113    }
114    for (int iw = 0; iw < N_times; iw++) { // for all frequencies

```

```

114     pow_spec[iw] *= normalization_factor;
115 }
116 }
117
118
119
120 void copy_mat (int M, int N, double mat_from[M][N], double mat_to[M][N]){
121     /* Copies matrix `mat_from` to `mat_to` */
122     for (int i = 0; i < M; i++) {
123         for (int j = 0; j < N; j++) {
124             mat_to[i][j] = mat_from[i][j];
125         }
126     }
127 }
128
129 void set_zero (int M, int N, double mat[M][N]){
130     /* Sets the matrix `mat` to zero */
131     for (int i = 0; i < M; i++) {
132         for (int j = 0; j < N; j++) {
133             mat[i][j] = 0;
134         }
135     }
136 }
137
138 void scale_mat (int M, int N, double mat[M][N], double alpha){
139     /* Scales the matrix `mat` by factor `alpha` */
140     for (int i = 0; i < M; i++) {
141         for (int j = 0; j < N; j++) {
142             mat[i][j] *= alpha;
143         }
144     }
145 }

```

B Auxiliary

B.1 Makefile

```

1  CC = gcc
2  CFLAGS = -O3 -Wall -Wno-unused-result
3
4
5  LIBS = -lm -lgsl -lgslcblas
6
7  HEADERS = initfcc.h alpotential.h funcs.h fft_func.h
8  OBJECTS = initfcc.o alpotential.o funcs.o fft_func.o
9
10
11 %.o: %.c $(HEADERS)
12     $(CC) -c -o $@ $< $(CFLAGS)
13
14 all: Task1 Task2 Task3 main_Prod.c
15
16 Task1: $(OBJECTS) main_T1.c
17     $(CC) -o $@ $^ $(CFLAGS) $(LIBS)
18
19 Task2: $(OBJECTS) main_T2.c
20     $(CC) -o $@ $^ $(CFLAGS) $(LIBS)
21
22 Task3: $(OBJECTS) main_T3.c
23     $(CC) -o $@ $^ $(CFLAGS) $(LIBS)
24
25 Prod: $(OBJECTS) main_Prod.c
26     $(CC) -o $@ $^ $(CFLAGS) $(LIBS)
27
28 # $(PROGRAMS): $(OBJECTS) main_T1.c
29 #     $(CC) -o $@ $^ $(CFLAGS) $(LIBS)
30
31 clean:
32     rm -f *.o
33     touch *.c

```

C Matlab scripts

C.1 Analysis scripts for tasks 3-7: A1_energies.m

```

1 tmp = matlab.desktop.editor.getActive; %% cd to current path
2 cd(fileparts(tmp.Filename));
3 set(0, 'DefaultFigureWindowStyle', 'docked');

```



```

4 GRAY = 0.7*[0.9 0.9 1];
5 warning('off','MATLAB:handle_graphics:exceptions:SceneNode'); % interpreter ↩
6 warning
7 %% task 1: lattice energies
8 clc
9 energy_data = load('../data/lattice_energies.tsv');
10 a0 = energy_data(:,1);
11 v0 = a0.^3;
12
13 energy = energy_data(:,2);
14 figure(1);clf;
15 plot(v0,energy, 'xk');
16
17 start_v = 64;
18 end_v = 68;
19 indToInclude = (v0 > start_v) & (v0 < end_v);
20 p = polyfit(v0(indToInclude),energy(indToInclude),2);
21 hold on;
22
23 vvec = linspace(start_v, end_v);
24 plot(vvec, p(1)*vvec.^2 + p(2)*vvec + p(3), '-r');
25 xlim([64 68]);
26
27 v_min = -p(2)/(2*p(1));
28 a_min = v_min^(1/3);
29
30 ax = gca;
31 ax.YLim = [-13.45 -13.42];
32 h1 = plot(v_min*[1 1], ax.YLim, '--k'); % plot vertical line at v_min
33
34
35 ax.YTick = (-13.45:0.01:-13.42);
36 ylabel('$E_{\rm pot}$ [eV/unit cell]');
37 xlabel('$a_0^3$ [\AA^3]');
38 legend('data', 'quadratic fit', ['$V_{\rm eq}$ \approx \, $' num2str(round(v_min↩
39 ,2)) '\, \AA^3$'], ...
40 'location', 'southeast')
41 ax = gca; ax.Children = ax.Children(3:-1:1);
42 ImproveFigureCompPhys(gcf); h1.LineWidth = 2; setFigureSize(gcf, 300, 600);
43
44 %axis([63 68 ylim(1) 0]);
45 saveas(gcf, '../figures/potential_energy.eps', 'eps')
46
47 %% task 2: find a suitable timestep
48 clc;clf;
49 dt=[1e-2,5e-3,2e-3,1e-3];
50 figure(1);clf;figure(2);clf;
51 for i=1:4
52     T_data = load(sprintf('../data/temperature_dt-%0.0e_Task2.tsv',dt(i)));
53     E_data = load(sprintf('../data/total_energy_dt-%0.0e_Task2.tsv',dt(i)));
54     t = T_data(:,1);
55     T = T_data(:,2);
56     E = E_data(:,2);
57
58     t_eq=0.5;
59
60     fprintf('dt = %0.0e\n',dt(i));
61
62     T_avg=mean(T(t>t_eq));
63     T_std=std(T(t>t_eq));
64     fprintf('\tT = %0.2f +- %0.1f %%\n', T_avg, abs(T_std/T_avg)*100);
65
66     E_avg=mean(E(t>t_eq));
67     E_std=std(E(t>t_eq));
68     fprintf('\tE = %0.2f +- %0.1e %%\n', E_avg, abs(E_std/E_avg)*100);
69
70     figure(1)
71     plot(t, T); hold on;
72
73     %yyaxis right
74     figure(2)
75     plot(t, E);hold on;
76     ylim(E_avg*(1+0.001*[1,-1]));
77 end
78 for ifig = 1:2
79     figure(ifig);
80     h = legend(strcat({'$dt = $ '}, num2str(round(dt',4)) , ' ps'));
81     xlabel('$t$ [ps]');
82     if ifig ==1
83         ylabel('$T$ [K]')
84     else
85         ylabel('$E_{\rm tot}$ [eV/unit cell]');
86         ax = gca; ax.YTick = (-13:0.1:-10);
87         ax.YLim = [-12.6 -12.2];
88         %h.Location = 'best';
89     end
90     ImproveFigureCompPhys(gcf,'Linewidth', 2);setFigureSize(gcf, 400, 400);
91 end
92 saveas(1, '../figures/dt-scan-temperature.eps', 'eps')

```

```

93 saveas(2, '../figures/dt-scan-energy.eps', 'epsc')
94
95 %% task 3: temperature and pressure equilibration,
96 % and task4: test production pressure and temperature
97
98 clc; clf;
99 temps = [500 700 500 700];
100 temperatures_str = num2str([500;700]);
101 FILENAMES = [strcat({'../data/temp-'}, temperatures_str, '_pres-1_Task3.tsv');
102             strcat({'../data/temp-'}, temperatures_str, '_pres-1_Prod-test.tsv')];
103 bar = 6.2415e-07;
104 Kelvin_to_degC = -273.15;
105 t_eqs = [1 1 0.5 0.5]; % approximate equilibration time
106 N_average_points = 50;
107 dt = 5e-3;
108 tau_eqilibration = 100*dt;
109
110 for iFile = 1:numel(FILENAMES)
111     figure(iFile);clf;
112     data = load(FILENAMES{iFile});
113
114     t = data(:,1);
115     T = data(:,2)+Kelvin_to_degC;
116     P = data(:,3)/bar;
117
118     t_eq=t_eqs(iFile);
119
120     %fprintf('dt = %0.0e\n',dt(i));
121     T_avg=mean(T(t>t_eq));
122     T_std=std(T(t>t_eq));
123     fprintf('\tT = %0.2f +- %0.1f K\n', T_avg, abs(T_std));
124
125     P_avg=mean(P(t>t_eq));
126     P_std=std(P(t>t_eq));
127     fprintf('\tP = %0.2f +- %0.1f bar\n', P_avg, abs(P_std));
128
129     yyaxis left
130
131     if iFile <=2 % equilibration run, otherwise production
132         plot(t./tau_eqilibration,T, 'color', GRAY),hold on;
133         plot(t./tau_eqilibration, movmean(T,N_average_points),'-k')
134     else
135         plot(t,T, 'color', GRAY),hold on;
136         plot(t, cumsum(T)./(1:length(t)),'-k')
137     end
138     ylabel('$T \, [\mathrm{K}]$')
139
140     if iFile <=2 % equilibration run, otherwise production
141         ylim(temps(iFile)*(1+ 0.3*[-1,1.2]))
142         yyaxis right
143         plot(t./tau_eqilibration,P),hold on;
144         plot(t./tau_eqilibration, movmean(P,N_average_points),'-k')
145         legend('$\mathcal{T}$', 'mov avg', '$\mathcal{P}$', 'mov avg');
146         xlabel('$t/\tau_{\mathrm{eq}}$')
147         xlim([0 5])
148     else
149         ylim(temps(iFile)+ 100*[-3,3])
150         yyaxis right
151         plot(t,P),hold on;
152         plot(t, cumsum(P)./(1:length(t)),'-k')
153         legend('$\mathcal{T}$', 'cum avg', '$\mathcal{P}$', 'cum avg');
154         xlabel('$t$, [ps]')
155     end
156     ylabel('$P \, [\mathrm{bar}]$')
157     ylim([-100,400])
158     ImproveFigureCompPhys(gcf, 'linewidth', 3, 'LineColor', {'MYORANGE', GRAY, 'MYBLUE', GRAY});
159     setFigureSize(gcf, 400, 400);
160 end
161
162
163 saveas(1, '../figures/TP-eq-500.eps', 'epsc')
164 saveas(2, '../figures/TP-eq-700.eps', 'epsc')
165 saveas(3, '../figures/TP-prod-500.eps', 'epsc')
166 saveas(4, '../figures/TP-prod-700.eps', 'epsc')
167
168
169 %% determine displacements and MSD
170 temperatures_str = num2str([500;700]);
171 clc; clf;
172 figure(10); clf;
173 FILENAMES = strcat({'../data/temp-'}, temperatures_str, '_pres-1_displacements.↵
174                       tsv');
175 FILENAMES_Dyn = strcat({'../data/temp-'}, temperatures_str, '_pres-1↵
176                       _dynamicProperties.tsv');
177 FILENAMES_Pow = strcat({'../data/temp-'}, temperatures_str, '_pres-1_power-↵
178                       spectrum.tsv');
179 for iFile = 1:numel(FILENAMES)
180     figure(iFile); clf;
181     data = load(FILENAMES{iFile});

```

```

180 t = data(:,1);
181 dx = data(:,2:end);
182
183 plot(t, dx.^2); hold on;
184
185 data = load(FILENAMES_Dyn{iFile});
186 MSD = data(:,2);
187 vel_corr = data(:,3);
188 plot(t, MSD, 'k')
189
190 if iFile ==2 % liquid
191     tStart = 1;
192     D = MSD(t>tStart)./(6*t(t>tStart));
193     selfDiffusionCoeff = mean(D); % in  $\text{\AA}^2/\text{ps}$ 
194     plot(t, 6*t*selfDiffusionCoeff, ':');
195 end
196
197 leg = legend([strcat({'$n=$'}, num2str((1:size(dx,2)))]); '$\Delta_{\rm MSD}\leftarrow$
198     ]$']);
199 leg.Location='northwest';
200 xlabel('$t$ [ps]')
201 ylabel('$\Delta x^2$, [\rm \AA^2]$')
202 if iFile ==1
203     ylim([0 1.0]);
204 else
205     ylim([0 20]);
206 end
207 ImproveFigureCompPhys(gcf, 'Linewidth', 2);
208 ax = gca; ax.Children(1).LineWidth = 4;
209
210 figure(10)
211 plot(t, vel_corr/vel_corr(1), 'color', GRAY); hold on;
212 xlim([0 1])
213 end
214
215 % % velocity correlation
216 figure(10);clf; figure(11);clf;
217 n_average_points = 1;%30;
218 for iFile = 1:numel(FILENAMES)
219     data = load(FILENAMES_Dyn{iFile});
220     t = data(:,1);
221     vel_corr = data(:,3);
222
223     data = load(FILENAMES_Pow{iFile});
224     freq = data(:,1);
225     pow_spec = data(:,2);
226
227     figure(10);
228     plot(t, vel_corr/vel_corr(1)); hold on;
229
230     dt = t(2)-t(1);
231     N_times = round(length(t)/2); % we have too bad statistics at later times.
232     deltaf = 1/(N_times * dt);
233     freqvec = 0:deltaf:(1/(2*dt));
234     PhiHat = 2 * trapz(t(1:N_times), (vel_corr(1:N_times) * ones(size(freqvec)))\leftarrow
235         .* cos(2*pi*t(1:N_times) * freqvec ), 1); %dimension 1
236     %PhiHat = 1/2 * 1/N_times * 2 * sum( (vel_corr(1:N_times) * ones(size(\leftarrow
237         freqvec))) .* cos(2*pi*t(1:N_times) * freqvec ), 1); %dimension 1
238
239     figure(11);
240     plot(freqvec, PhiHat); hold on;
241     plot(freq, pow_spec*t(end), ':'); hold on;
242     if iFile ==2 % liquid
243         tStart = 1;
244         selfDiffusionCoeff_spectral = PhiHat(1)/6; % in  $\text{\AA}^2/\text{ps}$ 
245     end
246 end
247
248 disp([selfDiffusionCoeff selfDiffusionCoeff_spectral]);
249
250 figure(10)
251 xlim([0 1])
252 leg = legend(strcat({'$T=$'}, num2str([500;700]), '\, '\circ $C'));
253 leg.Location='northeast';
254 xlabel('$t$ [ps]')
255 ylabel('$\Phi(t)/\Phi(0)$')
256 ImproveFigureCompPhys(gcf);
257
258 figure(11)
259 leg = legend('$T= 500 \, \, \circ \, C$, $ \hat{v} \, \Phi$', '$T= 500 \, \, \circ \, C$, $|\hat{v}|^2$',...
260     '$T= 700 \, \, \circ \, C$, $ \hat{v} \, \Phi$', '$T= 700 \, \, \circ \, C$, $|\hat{v}|^2$');
261 xlim([0 30])
262 ylim([0 Inf])
263 ImproveFigureCompPhys(gcf, 'LineColor', {'r', 'MYRED', 'GERIBLUE', 'MYLIGHTBLUE'\leftarrow
264     }');

```

C.2 Improve figure appearance: ImproveFigureCompPhys.m

```
1 function ImproveFigureCompPhys(varargin)
2 %ImproveFigureCompPhys Improves the figures of supplied handles
3 % Input:
4 % - none (improve all figures) or handles to figures to improve
5 % - optional:
6 %     LineWidth int
7 %     LineStyle column vector cell, e.g. {'-','--'}',
8 %     LineColor column vector cell, e.g. {'k',[0 1 1], 'MYBLUE'}'
9 %           colors: MYBLUE,MYORANGE,MYGREEN,MYPURPLE, MYYELLOW,
10 %           MYLIGHTBLUE, MYRED
11 %     Marker column vector cell, e.g. {'.', 'o', 'x'}'
12
13 % ImproveFigure was originally written by Adam Stahl, but has been heavily
14 % modified by Linnea Hesslow
15
16
17 %%% Handle inputs
18 % If no inputs or if the first argument is a string (a property rather than
19 % a handle), use all open figures
20 if nargin == 0 || ischar(varargin{1})
21     %Get all open figures
22     figHs = findobj('Type','figure');
23     nFigs = length(figHs);
24 else
25     % Check the supplied figure handles
26     figHs = varargin{1};
27     figHs = figHs(ishandle(figHs) == 1); %Keep only those handles that are ←
28     % proper graphics handles
29     nFigs = length(figHs);
30 end
31
32 % Define desired properties
33 titleSize = 24;
34 interpreter = 'latex';
35 lineWidth = 4;
36 axesWidth = 1.5;
37 labelSize = 22;
38 textSize = 20;
39 legTextSize = 18;
40 tickLabelSize = 18;
41 LineColor = {};
42 LineStyle = {};
43 Marker = {};
44
45 % define colors
46 co = [ 0      0.4470  0.7410
47       0.8500  0.3250  0.0980
48       0.9290  0.6940  0.1250
49       0.4940  0.1840  0.5560
50       0.4660  0.6740  0.1880
51       0.3010  0.7450  0.9330
52       0.6350  0.0780  0.1840 ];
53 colors = struct('MYBLUE', co(1,:),...
54               'MYORANGE', co(2,:),...
55               'MYYELLOW', co(3,:),...
56               'MYPURPLE', co(4,:),...
57               'MYGREEN', co(5,:),...
58               'MYLIGHTBLUE', co(6,:),...
59               'MYRED',co(7,:),...
60               'GERIBLUE', [0.3000  0.1500  0.7500],...
61               'GERIRED', [1.0000  0.2500  0.1500],...
62               'GERIYELLOW', [0.9000  0.7500  0.1000],...
63               'LIGHTGREEN', [0.4  0.85  0.4],...
64               'LINNEAGREEN', [7 184 4]/255);
65
66 % Loop through the supplied arguments and check for properties to set.
67 for i = 1:nargin
68     if ischar(varargin{i})
69         switch lower(varargin{i}) %Compare lower case strings
70             case 'linewidth'
71                 lineWidth = varargin{i+1};
72             case 'linestyle'
73                 LineStyle = varargin{i+1};
74             case 'linecolor'
75                 LineColor = varargin{i+1};
76                 for iLineColor = 1:numel(LineColor)
77                     if isfield(colors, LineColor{iLineColor})
78                         LineColor{iLineColor} = colors.(LineColor{iLineColor});
79                     end
80                 end
81             case 'marker'
82                 Marker = varargin{i+1};
83         end
84     end
85 end
86 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```

86
87 %% Improve the figure(s)
88
89 for iFig = 1:nFigs
90     fig = figHs(iFig);
91
92     lineObjects = findall(fig, 'Type', 'line');
93     textObjects = findall(fig, 'Type', 'text');
94     axesObjects = findall(fig, 'Type', 'axes');
95     legObjects = findall(fig, 'Type', 'legend');
96     contourObjects = findall(fig, 'Type', 'contour'); % not counted as lines
97
98     %% TEXT APPEARANCE: first set all to textSize and then change the ones
99     %% that need to be changed again
100
101     %Change size of any text objects in the plot
102     set(textObjects, 'FontSize', textSize);
103     set(legObjects, 'FontSize', legTextSize);
104
105     %% FIX LINESTYLE, COLOR ETC. FOR EACH PLOT SEPARATELY
106     for iAx = 1:numel(axesObjects)
107         lineObjInAx = findall(axesObjects(iAx), 'Type', 'line');
108
109         %set line style and color style (only works if all figs have some
110         %number of line plots..)
111         if ~isempty(LineStyle)
112             set(lineObjInAx, {'LineStyle'}, LineStyle)
113             set(contourObjects, {'LineStyle'}, LineStyle); %%%%%%%%%
114         end
115         if ~isempty(LineColor)
116             set(lineObjInAx, {'Color'}, LineColor)
117             set(contourObjects, {'LineColor'}, LineColor); %%%%%%%%%
118         end
119         if ~isempty(Marker)
120             set(lineObjInAx, {'Marker'}, Marker)
121             set(lineObjInAx, {'Markersize'}, num2cell(10+22*strcmp(Marker, '.'))←
122                 )
123         end
124
125         %%% change font sizes.
126         % Tick label size
127         xLim = axesObjects(iAx).XLim;
128         axesObjects(iAx).FontSize = tickLabelSize;
129         axesObjects(iAx).XLim = xLim;
130         %Change label size
131         axesObjects(iAx).XLabel.FontSize = labelSize;
132         axesObjects(iAx).YLabel.FontSize = labelSize;
133
134         %Change title size
135         axesObjects(iAx).Title.FontSize = titleSize;
136     end
137
138     %% LINE APPEARANCE
139     %Change line thicknesses
140     set(lineObjects, 'LineWidth', lineWidth);
141     set(contourObjects, 'LineWidth', lineWidth);
142     set(axesObjects, 'LineWidth', axesWidth)
143
144     % set interpreter: latex or tex
145     set(textObjects, 'interpreter', interpreter)
146     set(legObjects, 'Interpreter', interpreter)
147     set(axesObjects, 'TickLabelInterpreter', interpreter);
148 end
149 end

```

C.3 Change size of figures: setFigureSize.m

```

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

```