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4 Monte Carlo simulation of Hard spheres in the NVT ensemble (correct)

4.1

Here we had to make code that tiled the space with spheres in a cubic lattice formation. The code for the generation of this lattice is found in Appendix A.1.

On the web app for plotting this lattice, Figure 1 was made using the file that was generated.

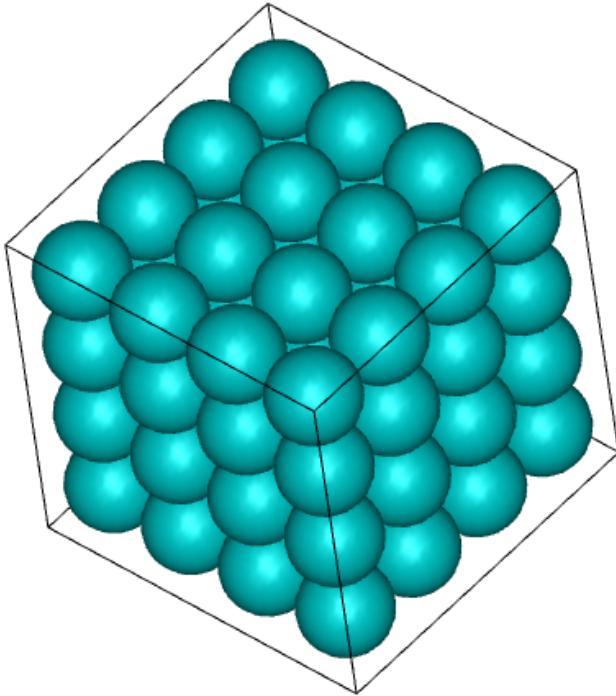


Figure 1: Here the cubic lattice generated by the code is graphed

4.2

We want to know the maximum packing density for spheres in a cubic lattice.

To get this first we need the lattice vector equation

$$\vec{R} = N_1 \vec{a}_1 + N_2 \vec{a}_2 + N_3 \vec{a}_3. \quad (1)$$

Here the $N_i \in \mathbb{Z}$ is the counting number and \vec{a}_i are the primitive translation vectors.

For the cubic case the vectors are unit vectors times the radius of the atoms. Dividing this up into unit cells gives us that only one atom may exist in the unit cell. meaning that the occupied fraction

$$f_o = \frac{V_p}{V_{uc}} = \frac{\frac{4}{3}\pi(\frac{a}{2})^3}{a^3} = \frac{\pi}{6} \quad (2)$$

Here V_p is the volume of particles occupying the unit cell, V_{uc} is the volume of the unit cell and a is the diameter of the particle.

4.3

Here we had to make code that tiled a space with spheres in a face-centered cubic (FCC) lattice. The code for the generation of this lattice is found in Appendix A.2.

On the web app for plotting this lattice, Figure 2 was made using the file that was generated.

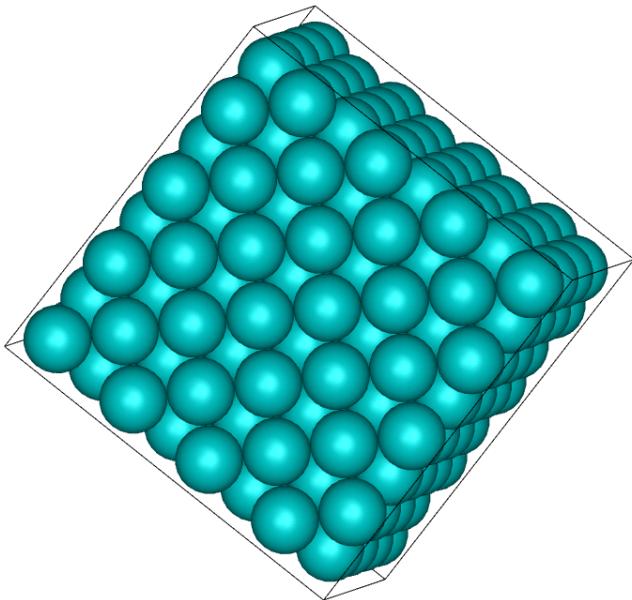


Figure 2: Here the cubic lattice generated by the code is graphed

4.4

We want to know the maximum packing density for spheres in a FCC lattice.

to get this we will use the same process as in 4.2. We know that our primitive translation vectors are

$$a_1 = \frac{a}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad a_2 = \frac{a}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad a_3 = \frac{a}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

If we do this we have a problem, choosing the unit cell with length a in each direction leads to a non-translation symmetric unit cell. To get a translation symmetric unit cell we have to chose the length of the unit cell to be $\sqrt{2}a$.

Looking at the unit cell we can see that for each corner 1/8th of a sphere exists and we get 1/2 for each face of the cube, meaning the cube contains $8 * 1/8 + 6 * 1/2 = 4$ spheres

From this we know that if we look at how much particles would be in a unit cell we see that this would be

$$f_o = \frac{4V_p}{V_{uc}} = \frac{\frac{16}{3}\pi(\frac{a}{2})^3}{(\sqrt{2}a)^3} = \frac{\pi}{3\sqrt{2}} \quad (3)$$

4.5

The code for this *read_data()* subroutine is found in Appendix A.4.

we first initialize the file that we are interested in, we then open the file and scan the first line. The first line contains the code number of particles in the system using which we know how much of the file we need to read. Then we have a line of code to read out the 3 box dimensions that are defined. After this we know the file contains (x,y,z,r) where the x,y,z are the coordinates and the r is the radius of the box. We read these putting x,y,z into the "r" vector (1D pointer) and r into the "size" vector (1D pointer).

4.6

The code for this *move_particle()* subroutine is found in Appendix A.6.

First we generate a random particle index for our position pointer.

Then a random amplitude for our translation is generated in the domain [-delta,delta]. After a random translation direction in 3D is generated, which is then normalised and scaled by the amplitude of the translation.

This translation is validated using the move *check_particle_overlap()* if it is found to not overlap the translation is executed.

After the translation we look if the particle is still in the box. If it is not the periodic boundaries are imposed.

4.7

The code for this *check_particle_overlap()* subroutine is found in Appendix ??.

It just tests that the random particle can do the translation without overlapping. This is done by checking its distance to all other particles and seeing if their radius's added are smaller then their distance.

4.8

The results of this NVT ensemble evolution of a cubic lattice are plotted in Figure 3.

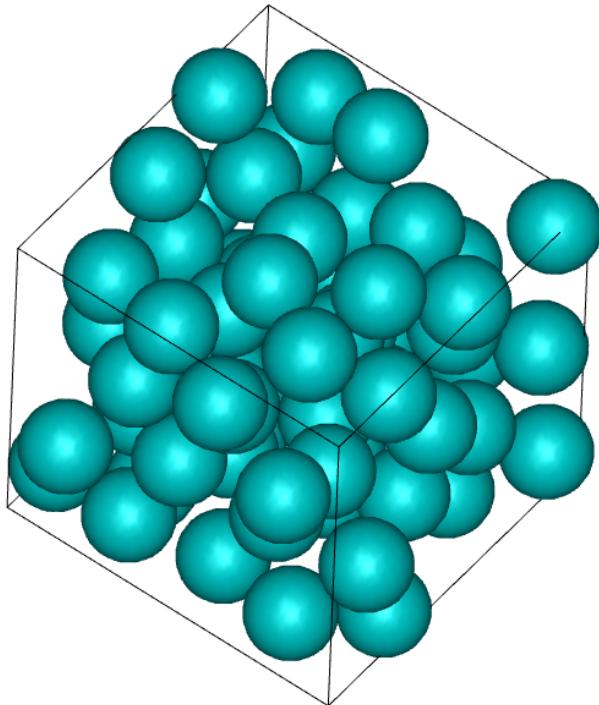
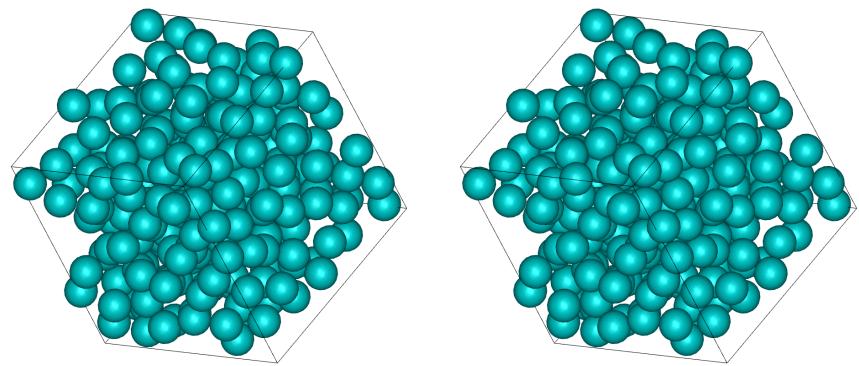


Figure 3: Here the cubic lattice generated is perturbed 100000 times to give this configuration

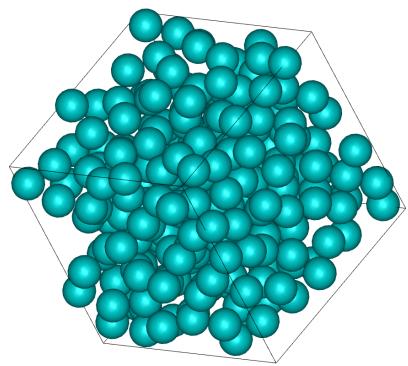
4.9

Figure 4 shows the NVT simulation at different packing densities.

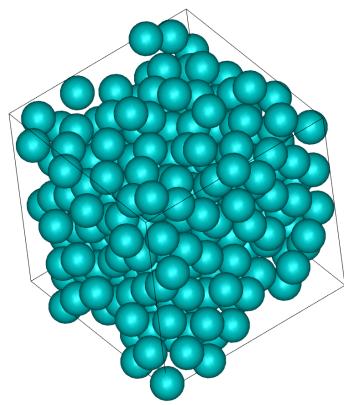
At a density .55 the particles still seem to have some underlying structure, while at a density of .4 it doesn't seem to have any underlying structure, with .5 and .45 its hard to tell, so somewhere in between the structure disappears meaning it melts in the range [.4 - .55].



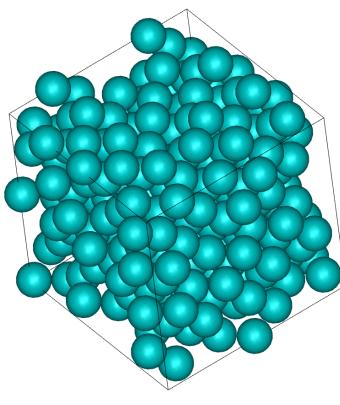
(a) the packing density is 0.40



(b) the packing density is 0.45



(c) the packing density is 0.50



(d) the packing density is 0.55

Figure 4: The packing density changed

5 MC simulation of hard spheres in the NPT ensemble

5.1

here we are asked to make a change volume to see if we have some overlap. The code for this part is found in Appendix B.1

A Code Exercise 4

A.1

```
1 #include <stdio.h>
2 #include <math.h>
3 // in this file we will make the cubic lattice
4
5 int main(){
6     int N = 4; // The number of particles in each direction
7     float d = 1.0; // the distance between two spheres
8     float a = 1.0; // the radius of an sphere
9
10    // Make a file where we can save the position data
11    FILE *print_coords; // initialises a file variable
12    print_coords = fopen("cubic_xyz.dat","w"); // defining the file variable to be the opening
13        of some file cubic.xyz
14
15    // Let us print some initial coordinates
16    fprintf(print_coords, "%i\n", N*N*N); // the total number of particles
17    fprintf(print_coords, "%lf\t%lf\n", -0.0, 1.0*d*N); // The occupied space in the x direction
18    fprintf(print_coords, "%lf\t%lf\n", -0.0, 1.0*d*N); // The occupied space in the y direction
19    fprintf(print_coords, "%lf\t%lf\n", -0.0, 1.0*d*N); // The occupied space in the z direction
20
21    // we first initialise the particle possision saving arrays
22    float x[N*N*N], y[N*N*N], z[N*N*N], r[N*N*N];
23
24
25    // now we start generating particle possisions and radiuses
26    int n = 0; // this is our counting variable, it wil index which particle we will consider
27
28    /*
29    The lattice points are described by
30    R= a_x n_x + a_y n_y + a_z n_z
31    a_x = i a
32    a_y = j a
33    a_z = k a
34    */
35
36    // sweeping over the N_x particles
37    for(int i=0; i<N; i++){
38        // sweeping over the N_y particles
39        for(int j=0; j<N; j++){
40            // sweeping over the N_z particles
41            for(int k=0; k<N; k++){
42                // generating the possition for i,j,k lattice cite, also the radius of the particle
43                x[n] = (i+0.5)*d;
44                y[n] = (j+0.5)*d;
45                z[n] = (k+0.5)*d;
46                r[n] = a;
47
48                // saving the x,y,z possition and radius of the particle
49                fprintf(print_coords, "%lf\t%lf\t%lf\t%lf\n", x[n], y[n], z[n], r[n]);
50
51                n++;
52            }
53        }
54    }
55
56
57    fclose(print_coords);
58    return 0;
59 }
```

A.2

```
1 #include <stdio.h>
2 #include <math.h>
3 // in this file we will make the cubic lattice
4
5 int main(){
6     int N = 4; // The number of particles in each double
7     double d = 1.0; // the distance between two spheres
8     double a = 1.0; // the radius of an sphere
9
```

```

10 // creating an distance variable that makes less typing
11 double l = sqrt(2.0)*d;
12
13 // defining the size of the box that will be spanned
14 double x_max = N*l;
15
16 // defining a variable such that the outline of the box aligns with the border of the
17 // particles
18 double s = 0.5*d;
19
20 // Make a file where we can save the position data
21 FILE *print_coords; // initialises a file variable
22 print_coords = fopen("fcc.xyz","w"); // defining the file variable to be the opening of some
23 // file cubic.xyz
24
25 // Let us print some initial coordinates
26 // Let us print some initial coordinates
27 fprintf(print_coords, "%i\n", 4*N*N*N); // the total number of particles
28 fprintf(print_coords, "%lf\t%lf\n", 0, x_max); // The occupied space in the x direction
29 fprintf(print_coords, "%lf\t%lf\n", 0, x_max); // The occupied space in the y direction
30 fprintf(print_coords, "%lf\t%lf\n", 0, x_max); // The occupied space in the z direction
31
32 // we first initialise the particle possision saving arrays
33 double x[4*N*N*N], y[4*N*N*N], z[4*N*N*N], r[4*N*N*N];
34
35 // now we start generating particle possisions and radiuses
36 int n = 0; // this is our counting variable, it wil index which particle we will consider
37
38 /*
39 The lattice points are described by
40 R= a_1 n_x + a_2 n_y + a_3 n_z
41 a_1 = a/2 (j + k)
42 a_2 = a/2 (i + k)
43 a_3 = a/2 (i + j)
44 i, j, k are the unit vectors in x, y and z directions respectively (not the counts)
45 */
46
47 // sweeping over the N_x particles
48 for(int i=0; i<N; i++){
49     // sweeping over the N_y particles
50     for(int j=0; j<N; j++){
51         // sweeping over the N_z particles
52         for(int k=0; k<N; k++){
53             // generating the possition for i,j,k lattice cite, also the radius of the particle
54
55             // first we start on the base vector because we know this patern reapeats every 2*unit
56             // vector in each direction
57             x[n] = (i)*l;
58             y[n] = (j)*l;
59             z[n] = (k)*l;
60             r[n] = a;
61
62             // saving the x,y,z possition and radius of the particle
63             fprintf(print_coords, "%lf\t%lf\t%lf\t%lf\n", x[n], y[n], z[n], r[n]);
64
65             n++;
66
67             // here we will add the a_1 vector and make the same spacing
68             x[n] = (i)*l;
69             y[n] = (j+0.5)*l;
70             z[n] = (k+0.5)*l;
71             r[n] = a;
72
73             // saving the x,y,z possition and radius of the particle
74             fprintf(print_coords, "%lf\t%lf\t%lf\t%lf\n", x[n], y[n], z[n], r[n]);
75
76             n++;
77
78             // here we will add the a_2 vector and make the same spacing
79             x[n] = (i+0.5)*l;
80             y[n] = (j)*l;
81             z[n] = (k+0.5)*l;
82             r[n] = a;

```

```

83     // saving the x,y,z position and radius of the particle
84     fprintf(print_coords, "%lf\t%lf\t%lf\t%lf\n", x[n], y[n], z[n], r[n]);
85
86     n++;
87
88     // here we will add the a3 vector and continue the same spacing
89     x[n] = (i+0.5)*l;
90     y[n] = (j+0.5)*l;
91     z[n] = (k)*l;
92     r[n] = a;
93
94     // saving the x,y,z possition and radius of the particle
95     fprintf(print_coords, "%lf\t%lf\t%lf\t%lf\n", x[n], y[n], z[n], r[n]);
96
97     n++;
98
99
100
101
102     }
103 }
104
105
106
107
108 fclose(print_coords);
109 return 0;
110 }
```

A.3

```

1 #include <stdio.h>
2 #include <time.h>
3 #include <assert.h>
4 #include <math.h>
5 #include "../downloads/mt19937.h"
6
7 #ifndef M_PI
8 #define M_PI 3.14159265358979323846
9 #endif
10
11 #define NDIM 3
12
13 /* Initialization variables */
14 const int mc_steps = 10000;
15 const int output_steps = 100;
16 const double packing_fraction = 0.6;
17 const double diameter = 1.0;
18 const double delta = 0.1;
19 const char* init_filename = "FCC_xyz.dat";
20
21 /* Simulation variables */
22 int N;
23 int n_particles = 0;
24 double radius;
25 double particle_volume;
26 double (*r)[3];
27 double *size;
28 double box[NDIM];
29
30
31 double dummy;
```

A.4

```

1 void read_data(void){
2     /*----- Your code goes here -----*/
3     // degining the file
4     FILE *read_cords;
5     read_cords = fopen(init_filename, "r");
6
7     // reading the first line to get the number of particles that exist in the file (why is
8     // the exersise so weird??)
9     fscanf(read_cords, "%i\n", &N); // the total number of particles
// printf("%i\n", Loaded_Data.N);
```

```

10 // making sure that the size will be correctly defined instead of having to assign it
11 // before hand
12 // malloc is the memory allocation command which is what we need to have exact size
13 // matrixes, only this satisfies me
14 r = malloc(N * sizeof * r); // all the position vectors of all the particles
15 size = malloc(N * sizeof * size); //The size of all particles
16
17 // lets turn the above into a loop because i want to
18 for(int i = 0; i<3; i++){
19     fscanf(read_cords, "%f %f", &dummy, &box[i]);
20 }
21
22 // now that we have arrived at the particles lets be happy
23 for(int i = 0; i<N; i++){
24     fscanf(read_cords, "%f %f %f %f", &r[i][0], &r[i][1], &r[i][2], &size[i]);
25 }
26
27 fclose(read_cords);
28 }
```

A.5

```

1 int check_particle_overlap(int n){
2     double *p = r[n];
3
4     for(int i=0;i<n_particles;i++){
5         if(i==n){
6             continue;
7         }
8
9         double *p_c = r[i];
10        double distance_squared = 0;
11
12        for(int j=0;j<3;j++){
13            double difference = p[j] + dr[j] - (p_c[j]);
14            if(difference>0.5*box[j]){
15                difference -= box[j];
16            }
17            else if(difference<-0.5*box[j]){
18                difference += box[j];
19            }
20            distance_squared += difference*difference;
21        }
22
23        double sum_raduss = 0.5 * (size[i] + size[i]);
24
25
26
27        if (distance_squared < sum_raduss*sum_raduss){
28            // printf("%lf\t < \t %lf\n",distance_squared,sum_raduss*sum_raduss);
29            return 1;
30        }
31    }
32 }
33 // printf("accept\n");
34 return 0;
35 }
36 }
```

A.6

```

1 int move_particle(void){
2     n = floor(dsfmt_genrand()*n_particles);
3
4     for(int i=0;i<3;i++){
5         dr[i] = (dsfmt_genrand()-0.5) + 0.00001;
6     }
7     double delta_l=(dsfmt_genrand()-0.5)*2*delta + 0.00001;
8
9     double length = sqrt(dr[0]*dr[0] + dr[1]*dr[1] + dr[2]*dr[2]);
10    for(int i=0;i<3;i++){
11        dr[i] *= delta_l/length;
12    }
```

```
13 int disp = check_particle_overlap(n);
14
15 if(disp ==1){
16     return 0;
17 }
18 else if (disp==0){
19     for(int i=0;i<3;i++){
20         r[n][i] += dr[i];
21
22         if(r[n][i]<0){
23             r[n][i] +=box[i];
24         }
25         if(r[n][i]>box[i]){
26             r[n][i] -=box[i];
27         }
28     }
29     return 1;
30 }
31
32 }
33 }
```

B Exercise 5

B.1

```
1 int change_volume(){
2
3     dV = (dsfmt_genrand() - 0.5)*2*dV_m;
4
5     double V = box[0]*box[0]*box[0];
6
7     double mult_fac = cbrt(V+dV)/box[0];
8
9     double V_new=1;
10
11    for(int i=0; i<3; i++){
12        V_new *=box[i]*mult_fac;
13    }
14
15    double acc = fmin(1, exp(-betaP*dV + n_particles*log(V_new/V)));
16    if (dsfmt_genrand()>acc){
17        return 0;
18    }
19
20    double r_c[n_particles][3];
21
22    for(int i=0; i<n_particles; i++){
23
24        for(int j=0; j<3; j++){
25
26            r_c[i][j] = r[i][j] *mult_fac;
27        }
28    }
29
30    for(int h=0; h<n_particles; h++){
31
32        for(int i=0; i < h; i++){
33
34            double distance = 0;
35
36            for(int j=0; j<3; j++){
37
38                double dist = (r_c[h][j] - r_c[i][j]);
39
40                if(dist>0.5*box[j]*mult_fac){
41                    dist -= box[j]*mult_fac;
42                }
43                else if(dist<-0.5*box[j]*mult_fac){
44                    dist += box[j]*mult_fac;
45                }
46
47                distance += dist*dist;
48
49            }
50
51        }
52
53
54        if (distance<(0.5*(size[h]+size[i]))*(0.5*(size[h]+size[i]))){
55            // printf("volume cannot change there is overlap\n");
56            return 0;
57        }
58    }
59
60 }
61
62
63
64
65    for(int i=0;i<3;i++){
66        box[i]*=mult_fac;
67    }
68    for(int i=0; i<n_particles; i++){
69        for(int j=0; j<3; j++){
70            r[i][j] = r_c[i][j];
71        }
72    }
```

```

73 // printf("volume changed\n");
74 return 1;
75
76 }
77 }
```

B.2

```

1 int main(int argc, char* argv[]){
2     read_data();
3
4     assert(packing_fraction > 0.0 && packing_fraction < 1.0);
5     assert(diameter > 0.0);
6     assert(delta > 0.0);
7
8     radius = 0.5 * diameter;
9
10    if(NDIM == 3) particle_volume = M_PI * pow(diameter, 3.0) / 6.0;
11    else if(NDIM == 2) particle_volume = M_PI * pow(radius, 2.0);
12    else{
13        printf("Number of dimensions NDIM = %d, not supported.", NDIM);
14        return 0;
15    }
16
17
18
19
20    if(n_particles == 0){
21        printf("Error: Number of particles, n_particles = 0.\n");
22        return 0;
23    }
24
25    set_packing_fraction();
26
27    dprintf_seed(time(NULL));
28
29    int accepted = 0;
30    int step, n;
31    int ind =0;
32    int accepted_dv = 0;
33
34    for(step = 1; step < mc_steps; ++step){
35        for(n = 0; n < n_particles; ++n){
36            accepted += move_particle();
37        }
38        accepted_dv += change_volume();
39
40        if(step % output_steps == 0){
41
42            double acceptance_move = (double)accepted / (n_particles * output_steps);
43            double acceptance_vol = (double)accepted_dv / (output_steps);
44
45            printf("Step %d. Move acceptance: %lf.\n", step, acceptance_move);
46            printf("Step %d. Volume change acceptance: %lf.\n", step, acceptance_vol);
47
48            write_data(step);
49
50            if(converged_vol<4){
51                if (acceptance_vol>0.55){
52                    dV_m *= 1.1;
53                }
54                else if (acceptance_vol<0.45){
55                    dV_m *= 0.9;
56                }
57                else{
58                    converged_move =0;
59                    converged_vol++;
60                }
61            }
62        }
63
64        if(converged_move<4){
65            if (acceptance_move>0.55){
66                delta *= 1.1;
67            }
68        }
69    }
70
71    if(delta < 0.01)
72        break;
73
74    write_data(step);
75
76    if(acceptance_move > 0.55)
77        delta *= 1.1;
78
79    if(delta < 0.01)
80        break;
81
82    write_data(step);
83
84    if(acceptance_move > 0.55)
85        delta *= 1.1;
86
87    if(delta < 0.01)
88        break;
89
90    write_data(step);
91
92    if(acceptance_move > 0.55)
93        delta *= 1.1;
94
95    if(delta < 0.01)
96        break;
97
98    write_data(step);
99
100   if(acceptance_move > 0.55)
101      delta *= 1.1;
102
103   if(delta < 0.01)
104      break;
105
106   write_data(step);
107
108   if(acceptance_move > 0.55)
109      delta *= 1.1;
110
111   if(delta < 0.01)
112      break;
113
114   write_data(step);
115
116   if(acceptance_move > 0.55)
117      delta *= 1.1;
118
119   if(delta < 0.01)
120      break;
121
122   write_data(step);
123
124   if(acceptance_move > 0.55)
125      delta *= 1.1;
126
127   if(delta < 0.01)
128      break;
129
130   write_data(step);
131
132   if(acceptance_move > 0.55)
133      delta *= 1.1;
134
135   if(delta < 0.01)
136      break;
137
138   write_data(step);
139
140   if(acceptance_move > 0.55)
141      delta *= 1.1;
142
143   if(delta < 0.01)
144      break;
145
146   write_data(step);
147
148   if(acceptance_move > 0.55)
149      delta *= 1.1;
150
151   if(delta < 0.01)
152      break;
153
154   write_data(step);
155
156   if(acceptance_move > 0.55)
157      delta *= 1.1;
158
159   if(delta < 0.01)
160      break;
161
162   write_data(step);
163
164   if(acceptance_move > 0.55)
165      delta *= 1.1;
166
167   if(delta < 0.01)
168      break;
169
170   write_data(step);
171
172   if(acceptance_move > 0.55)
173      delta *= 1.1;
174
175   if(delta < 0.01)
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1190
1191   if(delta < 0.01)
1192      break;
1193
1194   write_data(step);
1195
1196   if(acceptance_move > 0.55)
1197      delta *= 1.1;
1198
1199   if(delta < 0.01)
1200      break;
1201
1202   write_data(step);
1203
1204   if(acceptance_move > 0.55)
1205      delta *= 1.1;
1206
1207   if(delta < 0.01)
1208      break;
1209
1210   write_data(step);
1211
1212   if(acceptance_move > 0.55)
1213      delta *= 1.1;
1214
1215   if(delta < 0.01)
1216      break;
1217
1218   write_data(step);
1219
1220   if(acceptance_move > 0.55)
1221      delta *= 1.1;
1222
1223   if(delta < 0.01)
1224      break;
1225
1226   write_data(step);
1227
1228   if(acceptance_move > 0.55)
1229      delta *= 1.1;
1230
1231   if(delta < 0.01)
1232      break;
1233
1234   write_data(step);
1235
1236   if(acceptance_move > 0.55)
1237      delta *= 1.1;
123
```

```

69     else if (acceptance_move<0.45){
70         delta *= 0.9;
71     }
72     else{
73         converged_move++;
74     }
75 }
76
77     inf[ind][2]=(double)acceptance_vol;
78     inf[ind][4]=(double)acceptance_move;
79     inf[ind][3]=(double)converged_vol;
80     inf[ind][5]=(double)converged_move;
81     inf[ind][0]=(double)step;
82     inf[ind][1]=(double)box[0]*box[0]*box[0];
83     ind++;
84
85
86
87
88     accepted = 0;
89     accepted_dv = 0;
90 }
91
92
93
94 }
95
96
97
98
99 info_2_file();
100
101 printf("done");
102 return 0;
103 }
```

B.3

```

1 void info_2_file(){
2     char new_name[128];
3     sprintf(new_name, "./data/data %i/info.dat", (int)floor(betaP));
4
5     FILE *print_coords; // initialises a file variable
6     // char *new_name = "info.dat";
7     print_coords = fopen(new_name,"w");
8
9     double size_average = 0;
10    for(int i = 0; i<n_particles;i++){
11        size_average += size[i];
12    }
13    size_average/=n_particles;
14
15    fprintf(print_coords, "%lf\t%lf\t%lf\t%lf\t%i\t%lf\n", delta, dV_m, betaP, n_particles,
16           size_average);
17
18    for(int i=0;i<output_steps;i++){
19
20        fprintf(print_coords, "%lf\t%lf\t%lf\t%lf\t%lf\t%lf\t%lf\t%lf\n", inf[i][0], inf[i][1],inf[i][2],inf
21 [i][3],inf[i][4],inf[i][5]);
22    }
23
24    fclose(print_coords);
25
26 }
```