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H2a: Binary Alloy

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Task N°	Points	Avail. points
Σ		

Introduction

Both the mean field theory and the Ising model play an important role in statistical mechanics. We use these two models to study a simple model of a binary alloy of 50 % copper and 50 % zinc, commonly known as brass. Some properties of the system can be easily determined in the mean field theory, but a numerical simulation of the Ising model gives more accurate results. Here, we compute various statistical properties and compare the results of the Ising model and the mean field theory.

In both the mean field theory and the Ising model, we model the binary alloy with a static, three-dimensional bcc lattice consisting of Cu and Zn atoms. Each atom has eight bonds to each nearest neighbor, with bond energies

$$\begin{aligned} E_{\text{CuZn}} &= -294 \text{ meV}, \\ E_{\text{CuCu}} &= -436 \text{ meV}, \\ E_{\text{ZnZn}} &= -113 \text{ meV}. \end{aligned} \quad (1)$$

Task 1: mean field theory

In the mean field theory (MFT) model, every individual atom is assumed to interact only with an average of the whole system, and the system is also assumed to be in equilibrium. All microscopic variations are therefore neglected.

In this binary alloy model, we have two sub-lattices (one Cu sub-lattice and one Zn sub-lattice) and we can define an order parameter

$$P = 2 \frac{\tilde{N}}{N} - 1, \quad (2)$$

where \tilde{N} is the number of Cu atoms in the Cu lattice and N is the total number of Cu atoms—equivalently, we could say that N is the number of lattice sites in the Cu sub-lattice and that \tilde{N}/N is the fraction of the atoms in the sub-lattice which are Cu. This order parameter can now be used to define the mean field theory of this system.

At first, we need a connection between the order parameter, P , and the temperature, T . To get to this we note that the equilibrium of the system is given by minimizing the Helmholtz's free energy, $F_{\text{MFT}} = U_{\text{MFT}} - TS_{\text{MFT}}$, where $U_{\text{MFT}} = E_{\text{MFT}}(P)$ is the system energy and $S_{\text{MFT}} = k_B \ln \omega_{\text{MFT}}$ is the entropy, where $\omega_{\text{MFT}} = \omega_{\text{MFT}}(P)$ is the number of possible micro-states. In the Cu sub-lattice, there are $\tilde{N} = (1 + P)N/2$ Cu atoms; therefore, the number of micro-states in the Cu sub-lattice is

$$\omega'_{\text{MFT}} = \binom{N}{\tilde{N}} = \frac{N!}{\tilde{N}!(N - \tilde{N})!} = \frac{N!}{[(1 + P)N/2]! [(1 - P)N/2]!} \quad (3)$$

and the entropy of the Cu sub-lattice is

$$\begin{aligned} S'_{\text{MFT}} &= k_B \ln \left(\frac{N!}{[(1 + P)N/2]! [(1 - P)N/2]!} \right) \\ &\approx Nk_B \ln(2) - k_B \frac{N}{2} [(1 + P) \ln(1 + P) + (1 - P) \ln(1 - P)], \end{aligned} \quad (4)$$

where Stirling's formula has been used to arrive at the last result. Now, the Zn sub-lattice is equivalent to the Cu sub-lattice but with the number Zn atoms and Cu atoms interchanged. The two lattices must therefore have the same entropies, and the full system entropy is just the sum of its parts; hence

$$S_{\text{MFT}} = 2Nk_B \ln(2) - Nk_B [(1 + P) \ln(1 + P) + (1 - P) \ln(1 - P)]. \quad (5)$$

Next, we need to find $E(P)$. Using the mean field approximation that every atom only interacts with the system average, we can derive the number of the different types of bonds. The number Cu-Cu bonds, $N_{\text{CuCu}}^{(\text{MFT})}$, are given by the number of Cu atoms in the Cu sub-lattice, \tilde{N} , times the number of bonds each atom has, 8, times the probability that another Cu atom is located in the Zn sub-lattice¹, $(N - \tilde{N})/N = (1 - P)/2$. This gives

$$N_{\text{CuCu}}^{(\text{MFT})} = 8 \frac{(1 + P)N}{2} \frac{1 - P}{2} = 2N(1 - P^2). \quad (6)$$

¹This is because bonds can only be made between atoms in different sub-lattices.

For the Zn-Zn bonds the number has to be the same, since the Zn and Cu atoms are interchangeable:

$$N_{\text{ZnZn}}^{(\text{MFT})} = N_{\text{CuCu}}^{(\text{MFT})} = 2N(1 - P^2). \quad (7)$$

Then we know that the total number of bonds in this system has to be $8N$, and therefore the remaining $8N - N_{\text{ZnZn}} - N_{\text{CuCu}}$ bonds has to be inter-species bonds:

$$N_{\text{CuZn}}^{(\text{MFT})} = 4N(1 + P^2). \quad (8)$$

The energy of the system is now given by

$$E_{\text{MFT}} = E_{\text{CuZn}} N_{\text{CuZn}}^{(\text{MFT})} + E_{\text{ZnZn}} N_{\text{ZnZn}}^{(\text{MFT})} + E_{\text{CuCu}} N_{\text{CuCu}}^{(\text{MFT})}, \quad (9)$$

which can be simplified to

$$E_{\text{MFT}}(P) = (E_0 - 2P^2 \Delta E)N \quad (10)$$

where

$$\begin{aligned} E_0 &= 2(E_{\text{CuCu}} + E_{\text{ZnZn}} + 2E_{\text{CuZn}}) = -2.274 \text{ eV}, \\ \Delta E &= (E_{\text{CuCu}} + E_{\text{ZnZn}} - 2E_{\text{CuZn}}) = 39 \text{ meV}, \end{aligned} \quad (11)$$

and where the bond energies are given in equation (1). We can now find the equilibrium $P = P_{\text{eq}}$ by minimizing the free energy

$$\begin{aligned} F_{\text{MFT}}(P, T) &= NE_0 - 2NP^2 \Delta E \\ &\quad - 2Nk_B T \ln(2) + Nk_B T \left[(P+1) \ln(1+P) + (1-P) \ln(1-P) \right] \\ &= NE_0 - N\Delta E \left(2P^2 + 2\bar{T} \ln(2) - \bar{T} \left[(P+1) \ln(1+P) + (1-P) \ln(1-P) \right] \right), \end{aligned} \quad (12)$$

where $\bar{T} = k_B T / \Delta E$.

The critical temperature

The critical temperature can be found by differentiating (12) with respect to P :

$$\begin{aligned} 0 &= \frac{\partial F_{\text{MFT}}(P, T)}{\partial P} \\ &= -4PN + N\bar{T} \left[\ln(1+P) + \frac{1+P}{1+P} - \ln(1-P) - \frac{1-P}{1-P} \right]. \end{aligned} \quad (13)$$

Equation (13) is always fulfilled for $P = 0$, which means that the free energy has a local extremum point at $P = 0 \forall \bar{T}$. By expanding (13) at small P , we find

$$0 = -4P + 2\bar{T}_{\text{crit}} P \rightarrow \bar{T}_{\text{crit}} = 2. \quad (14)$$

This means that $\bar{T}_{\text{crit}} = 2$ is the only extremum point at small P . We note that

$$\frac{\partial^2 F_{\text{MFT}}(P, T)}{\partial P^2} \Big|_{P=0} = 2N(\bar{T} - 2) \Rightarrow \begin{cases} P = 0 \text{ minimum if } \bar{T} > 2 \\ P = 0 \text{ maximum if } \bar{T} < 2. \end{cases} \quad (15)$$

Consequently, there is a phase transition $\bar{T} = \bar{T}_{\text{crit}} = 2$: the equilibrium order parameter $P \neq 0$ for $\bar{T} < 2$, whereas $P = 0$ for $\bar{T} > 2$.

Numerical calculations

To actually minimize (12) with respect to P for a given T , we need to employ numerical methods. We implemented this in MATLAB and used the `fminbnd` function to find the minimum in the range $P \in [0, 1]$. This would then give us P as a function of temperature, $P(T)$. With that, we can easily numerically calculate the system energy $U(T) = E(P(T))$ and heat capacity

$$C(T) = \frac{\partial U}{\partial T} = \frac{\partial E}{\partial P} \frac{\partial P}{\partial T}. \quad (16)$$

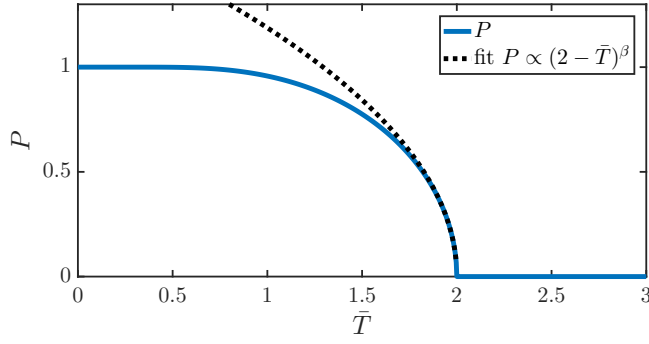


Figure 1: The mean field theory value of the order parameter, P , as a function of temperature, $\bar{T} = k_B T / \Delta E$. There is a clear critical temperature, $\bar{T}_{\text{crit}} = 2$ ($T_{\text{crit}} = 441$ K), above which P becomes constantly zero. Close below the critical temperature, there is a power law for $P(\bar{T}) \propto (\bar{T}_{\text{crit}} - \bar{T})^\alpha$, with $\alpha = 0.494$; this is shown as the black dotted line.

Results and discussion

From the numerical minimization of $F_{\text{MFT}}(P, T)$, we obtained $P(T)$ as shown in figure 1. There, we clearly see that there is a critical temperature at $\bar{T}_{\text{crit}} = 2$, which is consistent with the prediction (14). Numerically,

$$T_{\text{crit}} = \frac{2\Delta E}{k_B} = 441 \text{ K} = 168^\circ \text{C}. \quad (17)$$

Above this temperature the mean field theory predicts that $P(T > T_{\text{crit}}) = 0$ is constant, which corresponds to a maximally disordered system. Below the critical temperature P quickly rises to $P(0) = 1$, which is a maximally ordered system. Note, however, that the sign of P could just as well be flipped since the system is symmetric under the transformation $P \rightarrow -P$ (just switch label on which sub-lattice is which). There is a symmetry break at $T = T_{\text{crit}}$, below which the system will spontaneously order itself into an asymmetric state: $P < 0$ or $P > 0$.

We can also find an approximating power law near the critical temperature:

$$\hat{P}(T) \propto (\bar{T}_{\text{crit}} - \bar{T})^\beta = (2 - \bar{T})^\beta, \quad (18)$$

with a so called *critical exponent*, β . We used a log-log fit to find $\beta = 0.494$, and the corresponding power relation is shown as the dotted black line in figure 1.

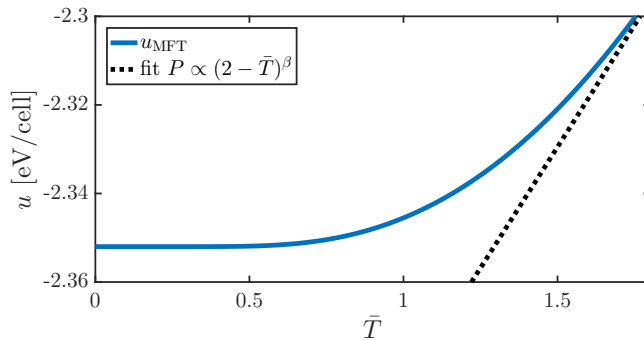


Figure 2: The mean field theory energy per unit cell, $u_{\text{MFT}} = U_{\text{MFT}}/N$, as a function of temperature, $\bar{T} = k_B T$. The energy rises from $u(\bar{T} = 0) = E_0 - 2\Delta E = -2.352$ eV to $u(\bar{T} = 0) = E_0 = -2.314$ eV per unit cell.

With $P(T)$ found, we can easily use (10) to find $U_{\text{MFT}}(T) = E_{\text{MFT}}(P(T))$, which is plotted in figure 2. There, we see that the energy rises with temperature, until we reach $\bar{T} = \bar{T}_{\text{crit}} = 2$ where, since P becomes constant $P = 0$, $U_{\text{MFT}}(T > T_{\text{crit}}) = NE_0 = -N \times 2.31$ eV becomes constant. We also see that using the corresponding power law (black dotted line) in $E(\hat{P})$ also agrees quite well.

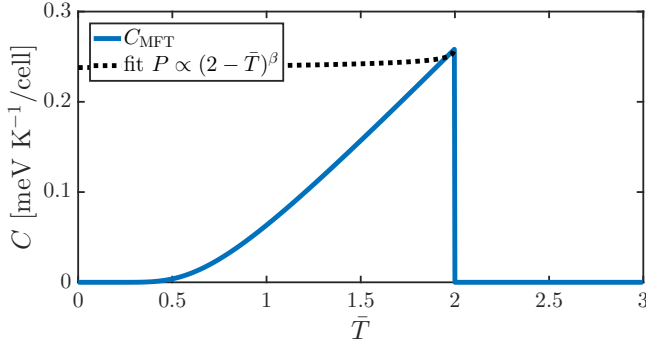


Figure 3: The mean field theory heat capacity, C_{MFT} , as function of temperature, $\bar{T} = k_B T / \Delta E$. The heat capacity rises until $\bar{T} = \bar{T}_{\text{crit}}$ to a maximum value of about $C_{\text{MFT}}^{(\text{max})} = 0.26 \text{ meV/K per unit cell}$, above which C_{MFT} immediately drops to 0.

Lastly, we can calculate the MFT heat capacity of the system by numerically differentiate U from before, the result of which is shown in figure 3. Here, we see an almost linear rise in heat capacity as T approaches T_{crit} . Then, above the critical temperature, the mean field theory heat capacity drops to $C_{\text{MFT}}(T > T_{\text{crit}}) = 0$. This is clearly not physical since that would mean that there is no cost in energy to change the temperature of the system above the critical temperature.

There is also a critical exponent for the heat capacity, $\hat{C} \propto (\bar{T}_{\text{crit}} - \bar{T})^{-\alpha}$. Using (16), we can easily show that

$$\hat{C} \propto (\bar{T}_{\text{crit}} - \bar{T})^{2\beta-1}, \quad (19)$$

which corresponds to $\alpha = 1 - 2\beta = 0.012$. This power law is also plotted in figure 3, but the agreement is much worse than in the previous two cases.

Task 2: Ising model

We use the Metropolis algorithm to estimate statistical properties of the system, which has a size of $10 \times 10 \times 10$ unit cells and periodic boundary conditions. In each simulation step, we swap two randomly selected atoms in the lattice, and determine the energy change ΔE . If

$$\Delta E \leq 0, \quad (20)$$

or if

$$\exp[-\Delta E / (k_B T)] > \xi, \quad (21)$$

where ξ is a random number between 0 and 1, the change is accepted; otherwise the lattice remains in the previous state for another step. In this way, the Metropolis algorithm allows us to sample the state space according to a probability $p \propto \exp[-E / (k_B T)]$, and thus favor the most probable configurations.

Equilibration

To equilibrate the system, we started with an ordered system and performed $N_{\text{eq,long}} = 10^6$ Monte Carlo steps to equilibrate the system at $T = -200^\circ\text{C}$. At higher temperatures, we started with the final lattice state of the previous temperature run, and therefore the number of equilibration steps was reduced to $N_{\text{eq,short}} = 5 \cdot 10^5$. For all temperatures, we used 10^7 Monte Carlo steps in the production run.

Figure 4 shows the equilibration of the energy at three different temperatures: significantly below, close to and significantly above the critical temperature $T \approx 430^\circ\text{C}$. We note that the energy per unit cell is in the range

$$E_0 - 2\Delta E \approx -2.35 \text{ eV} \leq E \leq E_0 \approx -2.27 \text{ eV}, \quad (22)$$

which is consistent with the mean field theory prediction (10); and the energy is equal to or lower than the completely random system where $E = E_0$.

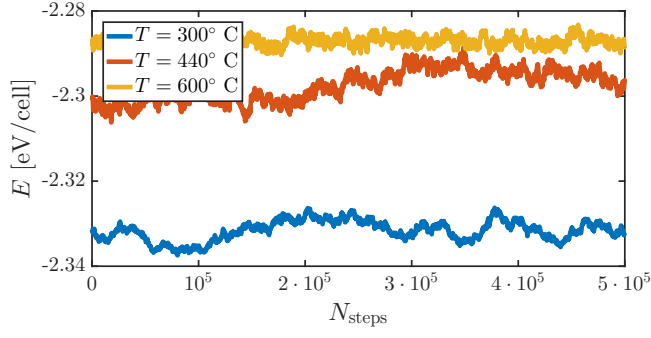


Figure 4: The energy per unit cell in the system during the equilibration process.

Statistical properties

Figure 5 shows the equilibrium energy per unit cell as a function of temperature, and compared to the mean field theory. We also show the error bars of two standard deviations using the statistical inefficiency as calculated from the correlation function in section .

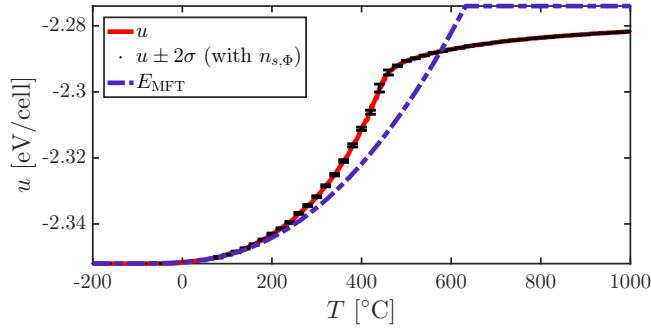


Figure 5: The average energy of the system normalized to the number of cells, as a function of temperature. Solid red: simulation, black: error bars at selected temperatures, dash-dotted blue: mean field theory prediction.

The metropolis simulation differs significantly from the mean free theory prediction: the critical temperature is significantly lower in the simulation, and the mean energy continues to increase with temperature beyond the transition. In mean field theory, the energy per unit in the range $u \in [E_0 - 2\Delta E, E_0]$ (see equation (22)). This is fulfilled also in the Monte Carlo simulation, which means that it did not develop clusters of Cu and Zn atoms, in which case the energy per bond would approach the average of the Cu-Cu and Zn-Zn bond energies. In contrast, the simulation does not reach the limit of $u = E_0$ even significantly above T_{crit} .

The heat capacity can be determined either by

$$C = \frac{\partial u}{\partial T}, \quad (23)$$

or as the variance in the energy:

$$C = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2). \quad (24)$$

Since the latter method does not depend on the derivatives, it gives less noisy data. This can be seen from figure 6 by comparing the gray and the black lines. Again, we note that the mean field theory gives a higher critical temperature than the simulation. Moreover, the heat capacity remains non-zero above the critical temperature. Thus, the Ising model does not share the unphysical artifact of the mean field theory (where there is no cost in energy to change the temperature of the system above the critical temperature). This is because the energy $u < E_0$ even at high temperatures in the simulation.

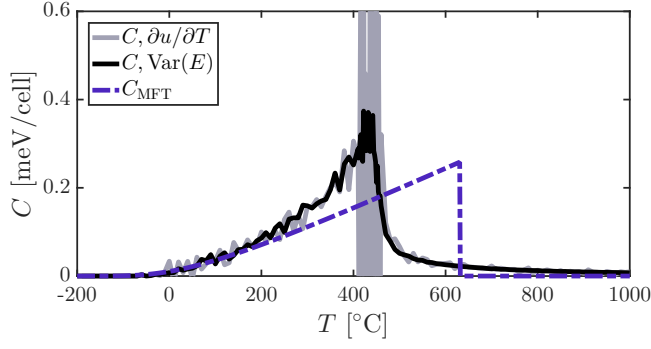


Figure 6: The specific heat of the system normalized to the number of cells, as a function of temperature. Solid gray: simulation using the derivative of U directly, black: simulation using the variance of E , dash-dotted blue: mean field theory prediction.

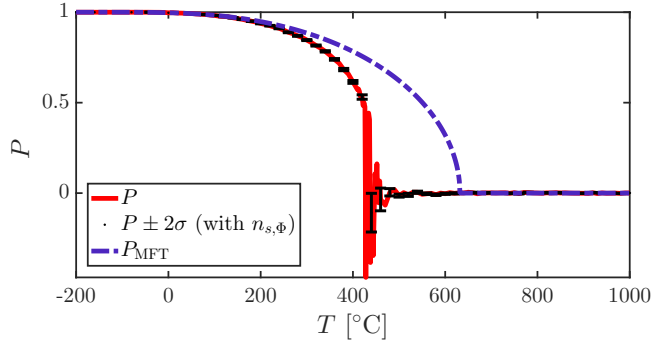


Figure 7: The order parameter P as a function of temperature. Solid red: simulation, black: error bars at selected temperatures, dash-dotted blue: mean field theory prediction.

The order parameter P is shown in figure 7. Close to the phase transition, the data has high uncertainty, which is also reflected in the large error bars. Note that $P < 0$ at some temperatures above the critical temperature – the system oscillates between a majority of the Cu atoms in the Cu sub-lattice, and a majority in the Zn sub-lattice.

Finally, the short range order parameter r is determined by the number of nearest-neighbor Cu-Zn bonds as follows

$$r = \frac{1}{4N}(N_{\text{CuZn}} - 4N) \rightarrow \begin{cases} 1, & \text{perfect order} \\ 0, & \text{no order, homogeneous system} \\ -1, & \text{fully separated system} \end{cases} \quad (25)$$

In the mean field theory,

$$r^{\text{MFT}} = \frac{1}{4N}[4N(1 + P^2) - 4N] = P^2 \quad (26)$$

by equation (8). Therefore, figure 8 shows not only the simulation and the MFT prediction, but also the curve P^2 . Until the transition, $r \approx P^2$ is a good estimation, but at higher temperatures r remains non-zero despite $P \approx 0$. This is a sign that there are still more Cu-Zn bonds than the completely random system. This is also consistent with the energy in figure 5, since

$$U = E_{\text{CuZn}}N_{\text{CuZn}} + \frac{1}{2}(8N - N_{\text{CuZn}})(E_{\text{ZnZn}} + E_{\text{CuCu}}) \quad (27)$$

$$= E_{\text{CuZn}}4N(r + 1) + 2N[1 - r](E_{\text{ZnZn}} + E_{\text{CuCu}}) \quad (28)$$

$$= NE_0 - 2Nr\Delta E. \quad (29)$$

Accordingly, $r = 0$ corresponds to the low temperature limit $u = E_0 - 2\Delta E$; the average energy then approaches $u \rightarrow E_0$ at high temperatures (c.f. equation (22)).

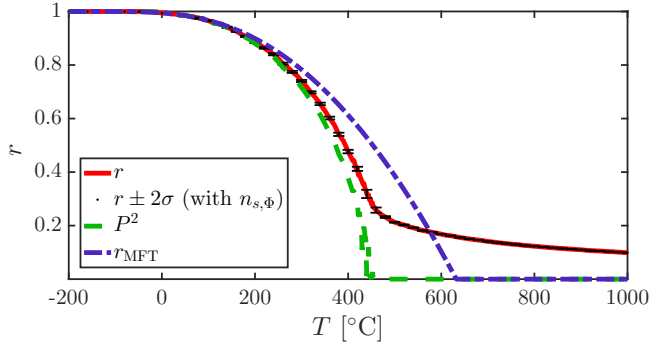


Figure 8: The short range order parameter as a function of temperature. Solid red: simulation, black: error bars at selected temperatures, dashed green: estimate $r \approx P^2$, dash-dotted blue: mean field theory prediction.

Finally a note on the critical exponents. Similarly to the MFT analysis, we performed a power law fit of the near-critical behavior of P and C , resulting in

$$\beta \approx 0.1, \quad \alpha \approx -0.2. \quad (30)$$

Although these values are highly uncertain, we note that the MFT prediction $\alpha_{\text{MFT}} = 1 - 2\beta_{\text{MFT}}$ does not generalize to the Ising model simulation.

Statistical inefficiency

As described in the Lecture notes, the statistical inefficiency can be used to obtain error estimates of correlated data.

Suppose we want to measure a quantity I , as an average of $N \gg 1$ measurements:

$$I = \langle f \rangle \equiv \frac{1}{N} \sum_{i=1}^N f_i. \quad (31)$$

The variance is then given by

$$\text{Var}[I] = \frac{n_s}{N} \text{Var}[f], \quad \text{Var}[f] = \langle f^2 \rangle - \langle f \rangle^2, \quad (32)$$

where n_s is the statistical inefficiency. The statistical inefficiency can be determined either from the decay of the correlation function,

$$\Phi_{k=n_s} = e^{-2} \approx 0.1, \quad \frac{\langle f_i f_{i+k} \rangle - \langle f \rangle^2}{\langle f^2 \rangle - \langle f \rangle^2}, \quad (33)$$

or from block averaging

$$n_s = \lim_{B \rightarrow \infty} \frac{B \text{Var}[F]}{\text{Var}[f]}, \quad F_j = \frac{1}{B} \sum_{i=1}^B f_{i+(j-1)B}, \quad j \in [1, N_{\text{blocks}}]. \quad (34)$$

The two methods in equations (33) and (34) should give similar estimates of n_s , which they do in the simulations here. The obtained statistical inefficiency is shown in figures 9 and 10 at three different temperatures, calculated with the correlation function and block average respectively.

In the case of block average, we used a moving average of 100 points, as the data become noisy when the block size become comparable to the total number of steps. Alternatively, we could have made more blocks of the largest sizes by also using shifted blocks of data, but the results obtained here were considered accurate enough.

Note in figures 9 and 10 that the statistical inefficiency is larger close to the phase transition at $T \approx 440^\circ\text{C}$ than at the lower and higher temperatures $T = 300^\circ\text{C}$ and $T = 600^\circ\text{C}$. We speculate that this is related to the diverging property of the correlation length close to the phase transition.

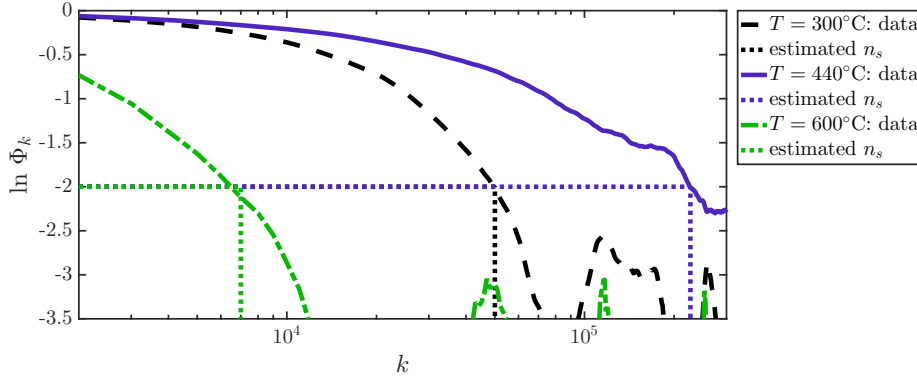


Figure 9: The logarithm of the correlation function $\Phi_k(k)$ for three different temperatures. Dotted lines mark the estimated value of $n_s = k(\ln \Phi_k = -2)$.

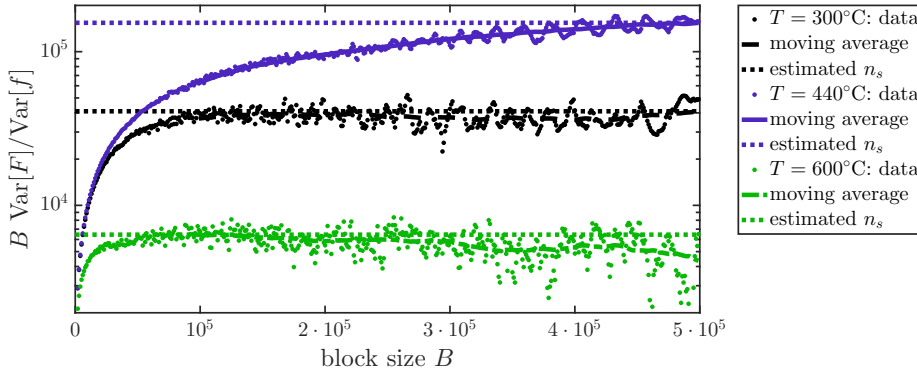


Figure 10: The statistical inefficiency determined with block averages for three different temperatures. Raw data is shown with dots, solid line show a moving average with 100 points, and the dotted lines show the estimated values of the statistical inefficiency.

This peak in the statistical inefficiency close to the phase transition can be clearly identified also in figure 11, where n_s is plotted as a function of temperature using the two methods described above. We note that both methods give consistent estimates of n_s , but the correlation function give larger fluctuations than the block average method. Moreover, that the statistical inefficiency diverges as $T \rightarrow 0$ K. This is because very few changes in the lattice will be accepted at low temperatures, resulting in highly correlated data. At low temperatures, the equilibrium system is almost completely ordered, and therefore the uncertainty of the quantities U , P and r is still small at low temperatures; note the vanishing $2 - \sigma$ error bars in figures 5-8.

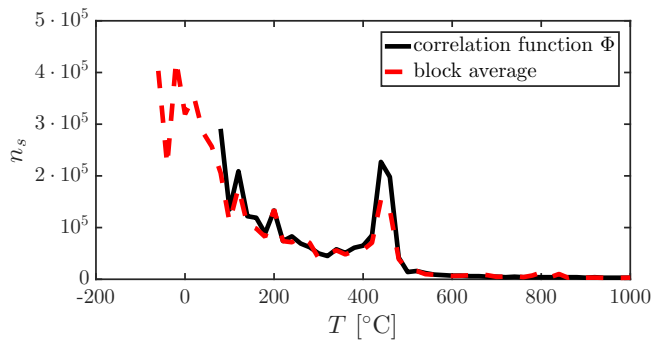


Figure 11: The statistical inefficiency n_s as a function of temperature using both the correlation function and block averages to determine n_s .

Concluding discussion

We study a binary alloy of brass. We compare semi-analytical results from mean-field theory with a Monte Carlo simulation using the Metropolis algorithm, and determine the energy, heat capacity, the order parameter as well as the short range order parameter.

We find that the mean field theory overestimates the critical temperature. Furthermore, it fails to explain the behavior of the system above this phase transition, as the simulations show a slower convergence to the high-temperature behavior. This results in a non-zero heat capacity at supercritical temperatures, as well as a non-zero short range order parameter r . We also determine the critical exponents associated with the order parameter P and the heat capacity from the simulations. Although these are uncertain, it is clear that they differ significantly from the mean field theory prediction.

Finally, we consider the statistical inefficiency. The block average method is consistent with the results using the correlation function, and we observe a peak in close to the phase transition, which is possibly connected to the longer correlation length of a system close to the phase transition.

A Source Code

A.1 Main program task 2: main.T2.c

```
1  /*
2   H2a, Task 2
3  */
4  #include <stdio.h>
5  #include <math.h>
6  #include <stdlib.h>
7
8  #include "funcs.h"
9
10 #define Nc 10 //number of cells
11 #define N_neigh 8
12 #define degC_to_K 273.15
13 #define kB 8.61733e-5
14
15 /* Main program */
16 int main(){
17     int N_Cu = Nc*Nc*Nc;
18     int N_atoms = 2*N_Cu;
19     int N_bonds = 8*N_Cu;
20     double Etot, E_Var, r, P; // Macro parameters
21     gsl_rng *q = init_random(); // initialize random number generator
22
23     /* done for all saved steps: */
24     int N_MCsteps = 1e7;
25     int N_eq = 1e6;
26     int N_eq_short = 5e5;
27     double *E_equilibration = malloc(sizeof(double[N_eq]));
28     double *P_equilibration = malloc(sizeof(double[N_eq]));
29     double *E_production = malloc(sizeof(double[N_MCsteps]));
30
31     /* statistical inefficiency */
32     int N_k = 500;
33     int N_skip = 1000; // k_Max = N_k * N_skip;
34     double *phi = malloc(sizeof(double[N_k]));
35     double *var_F = malloc(sizeof(double[N_k]));
36
37     /* set Temperature steps */
38     double beta;
39     double dT_small = 2;
40     double dT_large = 10;
41     double T_start = -200;
42     double T_end = 1000;
43     double T_start_fine = 410;
44     double T_end_fine = 460;
45     int nT;
46     double *T_degC = init_temps(&nT, dT_small, dT_large, T_start, T_end,
47                                T_start_fine, T_end_fine);
48     // save equilibration data and stat inefficiency at T%20 =0
49     int T_save_step = 20;
50     /* done for all temps: */
51     double *E_mean = malloc(sizeof(double[nT]));
52     double *E_mean_approx = malloc(sizeof(double[nT]));
53     double *E_sq_mean = malloc(sizeof(double[nT]));
54     double *P_mean = malloc(sizeof(double[nT]));
55     double *P_sq_mean = malloc(sizeof(double[nT]));
56     double *r_mean = malloc(sizeof(double[nT]));
57     double *r_sq_mean = malloc(sizeof(double[nT]));
58
59     /* allocate and initialize lattice and nearest neighbors */
60     int *lattice = malloc(sizeof(int[N_atoms]));
61     init_ordered_lattice(N_atoms, N_Cu, lattice);
62     int (*nearest)[N_neigh] = malloc(sizeof(int[N_atoms][N_neigh]));
63     init_nearestneighbor(Nc, nearest);
64
65     /* initialize macro parameters */
66     Etot = get_Etot(lattice, N_Cu, nearest);
67     P = get_order_parameter(lattice, N_Cu);
68     r = get_short_range_order_parameter(lattice, nearest, N_Cu);
69
70
71     /* ***** start simulation ***** */
72     for (int iT=0; iT<nT; iT++){
73         /* Loop over all temperatures */
74         printf("Now running T = %.0f degC\n", T_degC[iT]);
75         beta = 1/(kB*(T_degC[iT] + degC_to_K));
76
77         /* ***** Equilibration run ***** */
78         if (iT!=0){// First run needs longer equilibration
79             N_eq=N_eq_short;
80         }
81         /* Do the Monte Carlo stepping */
82         for( int i=0; i<N_eq; i++){
83             MC_step(&Etot, &r, &P, q, lattice, nearest, beta, N_Cu);
```

```

84 // Save the energy `Etot` and orerparameter `P`
85 E_equilibration[i] = Etot;
86 P_equilibration[i]= P;
87 }
88 //Write the equilibration run to file
89 if ( ((int)T_degC[iT]) % T_save_step==0){
90     write_equil_to_file(T_degC[iT],
91         E_equilibration, N_bonds, P_equilibration, N_eq);
92 }
93
94 /* ***** Production run ***** */
95 /*
96 The saved energies are shifted by this (semi-arbitrary) amount.
97 This helps to increase the accuracy when calculating the
98 (needed for the heat capacity).
99 */
100 E_mean_approx[iT] = Etot;
101 /* initialize at temperature[iT] */
102 E_mean[iT] = 0; E_sq_mean[iT] = 0;
103 P_mean[iT] = 0; P_sq_mean[iT] = 0;
104 r_mean[iT] = 0; r_sq_mean[iT]=0;
105
106 /* Do the Monte Carlo stepping */
107 for( int i=0; i<N_MCsteps; i++){
108     MC_step( &Etot, &r, &P, q, lattice, nearest, beta, N_Cu);
109     E_production[i] = Etot- E_mean_approx[iT];
110     update_E_P_r(iT, Etot-E_mean_approx[iT], E_mean, E_sq_mean, P, P_mean,
111         P_sq_mean, r, r_mean, r_sq_mean, lattice, nearest, N_Cu);
112 }
113 /* Divide by number of Monte Carlo steps to get average */
114 E_mean[iT] *= 1/((double)N_MCsteps);
115 E_sq_mean[iT] *= 1/((double)N_MCsteps);
116 P_mean[iT] *= 1/((double)N_MCsteps);
117 P_sq_mean[iT] *= 1/((double)N_MCsteps);
118 r_mean[iT] *= 1/((double)N_MCsteps);
119 r_sq_mean[iT] *= 1/((double)N_MCsteps);
120
121 /*
122 We only calucluate the statistical inefficiency at some
123 temperatures to save on runtime.
124 */
125 if ( ((int)T_degC[iT]) % T_save_step==0 ){//calc stat ineff
126     // Calcualte the variance of the energy
127     E_Var = E_sq_mean[iT] - E_mean[iT]*E_mean[iT];
128
129     printf("Calculating statistical inefficiencies \n");
130     //Calcualte the auto-correlation
131     get_phi (phi, N_MCsteps, E_mean[iT], E_Var, E_production, N_k, N_skip);
132     //Calcualte the block-average variance
133     get_varF_block_average(var_F, N_MCsteps, E_mean[iT], E_Var,
134         E_production, N_k, N_skip);
135     //Write the stat ineff to file
136     write_stat_inefficiency_to_file(T_degC[iT], phi, var_F, N_k, N_skip);
137 }//END if calc stat ineff
138 }//END temp for
139
140 //Write the results of the production run to file
141 write_production(T_degC, nT, E_mean_approx, E_mean, E_sq_mean,
142     P_mean, P_sq_mean, r_mean, r_sq_mean);
143
144
145
146 //Don't forget to free all malloc's.
147 free(nearest); nearest = NULL;
148 free(lattice); lattice = NULL;
149 free(E_equilibration); E_equilibration = NULL;
150 free(P_equilibration); P_equilibration = NULL;
151 free(E_mean); E_mean = NULL;
152 free(E_mean_approx); E_mean_approx = NULL;
153 free(E_sq_mean); E_sq_mean = NULL;
154 free(P_mean); P_mean = NULL;
155 free(P_sq_mean); P_sq_mean = NULL;
156 free(r_mean); r_mean = NULL;
157 free(r_sq_mean); r_sq_mean = NULL;
158 free(E_production); E_production = NULL;
159 free(phi); phi = NULL;
160 free(var_F); var_F = NULL;
161 free(T_degC); T_degC = NULL;
162
163 gsl_rng_free(q); // deallocate rng
164 return 0;
165 }

```

A.2 Misc functions : funcs.c

```
1 #include "funcs.h"
```

```

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```

/***** get functions *****/
double get_bond_E(int site_1, int site_2){
    /*
    The bond can be one of three types: ZnZn, CuZn=ZnCu, or CuCu.
    With the lattice encoding Cu=1 and Zn=0, we get
    Zn+Zn = 0, Zn+Cu = Cu+Zn = 1, Cu+Cu = 2.
    Hence the switch over the three cases: 0, 1, and 2.
    */
    double Ebond=0;
    switch (site_1 + site_2){
    case 0:
        Ebond= -0.113;//E_ZnZn;
        break;
    case 1:
        Ebond= -0.294;//E_CuZn;
        break;
    case 2:
        Ebond= -0.436;//E_CuCu;
        break;
    }
    return Ebond;
}

double get_order_parameter(int *lattice, int N_Cu){
    /*
    The macro order parameter 'P' is given by the number of atoms in
    their respective sub-lattice (normalized and shifted to get a
    better physical interpretation), e.g. the number of Cu atoms in
    the Cu sub-lattice.
    */
    int N_Cu_in_Cu_lattice=0;
    for(int i=0;i<N_Cu;i++){
        /*
        Sum the atoms in the Cu sub-lattice (i=0,1,2,...,N_Cu-1), and
        with the encoding Cu=1 and Zn=0, we can simply add the values
        of the lattice encoding at each sub-lattice point.
        */
        N_Cu_in_Cu_lattice+=lattice[i];
    }
    return (double)N_Cu_in_Cu_lattice/N_Cu *2 -1;
}

double get_short_range_order_parameter(int *lattice, int(*nearest)[N_neigh],
    int N_Cu){
    /*
    The short range order parameter 'r' is given by the number of AB bonds
    (normalized and shifted to get a better physical interpretation).
    */
    int N_CuZnBonds=0;
    for(int i=0;i<N_Cu;i++){
        for( int j=0; j<N_neigh; j++){
            /*
            With the encoding Cu=1 and Zn=0, we know that in order for a
            bond to be a CuZn/ZnCu the sum of a lattice point with its
            neighbour must be 1 (see 'get_bond_E' for more detail).
            */
            N_CuZnBonds+= ((lattice[i] + lattice[nearest[i][j]]) == 1);
        }
    }
    return (double) N_CuZnBonds/(4*N_Cu)-1; // this is 'r'
}

double get_Etot(int *lattice, int N_Cu, int (*nearest)[N_neigh]){
    /*
    The total energy of the system is given by looping over every atom
    in one of the sub-lattices (Cu) and summing the energies of its
    bonds to every neighbour.
    We only need to sum over every atom in one sub-lattice since there
    are no bonds within a sub-lattice.
    */
    double Etot=0;
    for(int i=0; i<N_Cu; i++){ // loop over atoms
        for( int j=0; j<N_neigh; j++){ // loop over neighbours
            Etot+= get_bond_E(lattice[i], lattice[nearest[i][j]]);
        }
    }
    return Etot;
}

void get_phi (double *phi, int N_times, double f_mean,
    double f_var, double *data, int N_k, int N_skip){
    /*
    Function for calculating the auto-correlation in a data set. The
    rate at which the auto-correlation decay can be used to calculate
    the statistical inefficiency in the data set.
    Formula:
    phi_k = (<f_{i+k}f_i> - <f_i>^2) / (<f_i>^2 - <f_i>^2)
    Note that, by definition, phi_0 = 1.
    */

```

```

93 int N_terms_in_avg; // helper variable
94 for (int k=0; k<N_k; k++){
95     /*
96     We loop over `k` in the formula above to get the auto-correlation
97     at the different times.
98     `phi[k]` is used to hold intermediary values, and only becomes the
99     auto-correlation at the last step in this loop.
100    */
101    phi[k] = 0;
102
103    /*
104    The number of terms in the sum to get  $\langle f_{i+k} f_i \rangle$  must be such
105    that i fulfills the relation:
106    `(i+k)*N_skip < N_times`,
107    which is equivalent to saying that
108    `i < N_times/N_skip - k`.
109    */
110    N_terms_in_avg = N_times/N_skip - k;
111    for (int i=0; i<N_terms_in_avg; i++){
112        /*
113        Add the products of the off-setted data points to get:
114        sum_{i} f_{i+k}f_{i}
115        */
116        phi[k] += data[i*N_skip]*data[(i+k)*N_skip];
117    }
118    /*
119    First:
120     $\langle f_{i+k} f_i \rangle = (1/N\_avg) \sum_{i} \{N\_avg\} f_{i+k} f_i$ ,
121    then we get the auto-correlation by subtracting `f_mean`^2
122    and dividing by the variance.
123    */
124    phi[k] = (phi[k]/N_terms_in_avg - f_mean*f_mean)/f_var;
125 }
126 }
127
128 void get_varF_block_average(double *var_F, int N_times, double f_mean,
129                             double f_var, double *data, int N_k, int N_skip){
130     /*
131     Function for calculating the variances of the blockaverages for `N_k`
132     different block sizes. This variance can then be used to calculate the
133     statistical inefficiency in the data set.
134     */
135     int block_size;
136     double Fj; // help variable, holding each block average
137     int number_of_blocks; // The number of blocks depends on the block size
138
139     for (int k=0; k<N_k; k++) { // block size loop
140         /*
141         For every block size, we need to loop over every block,
142         and every element in that block
143         */
144         block_size = N_skip * (k+1);
145         number_of_blocks = N_times/block_size;
146
147         var_F[k] = 0; // start
148         for (int j=0; j<number_of_blocks; j++) { // loop over all blocks
149             /* For every block, we loop over all elements in it to take average. */
150             Fj = 0; // reset to 0
151             for (int i=0; i<block_size; i++) { // internal block loop
152                 /* Adding all elems in the block to get the average */
153                 Fj += data[j*block_size + i];
154             }
155             Fj *= 1/(double)block_size; // divide by block size to get average
156             var_F[k] += Fj*Fj; // will become the variance soon
157         }
158         /*
159         To get the variance of F we use:
160          $Var[F] = \langle F^2 \rangle - \langle F \rangle^2 = \langle F^2 \rangle - \langle f \rangle^2$ ,
161         where f is the data set the block averages were taken from.
162         */
163         var_F[k] = var_F[k]/number_of_blocks - f_mean*f_mean;
164         var_F[k] *= block_size/f_var;
165     } // end block size loop
166 }
167
168 /***** Monte Carlo step functions *****/
169 void MC_step( double *Etot, double *r, double *P, gsl_rng *q,
170              int *lattice, int (*nearest)[N_neigh], double beta, int N_Cu){
171     /*
172     Function that takes a Monte Carlo step and updates the lattice points,
173     `Etot`, `r`, and `P` accordingly.
174     It is important to utilize the _chage_ in energy, `r` and `P` when
175     updating them as to not have to do a costly full calculation of either
176     every step in the Monte Carlo loop.
177     */
178     // Picks two random sites in the whole lattice.
179     int i1 = (int)(2*N_Cu*gsl_rng_uniform(q));
180     int i2 = (int)(2*N_Cu*gsl_rng_uniform(q));
181     // saves the original values
182     int old_1 = lattice[i1];
183     int old_2 = lattice[i2];

```

```

184 // Used to calculate the change in `Etot` and `r`
185 double dr = 0;
186 double dE = 0;
187 // We only need to do something if the two atoms are different
188 if (old_1 != old_2){
189     for( int j=0; j<N_neigh; j++){
190         /*
191          The change in `Etot` and `r` are first _minus_ the old energies and `r`
192          contributions.
193          */
194         dE -= get_bond_E(lattice[i1], lattice[nearest[i1][j]])
195             + get_bond_E(lattice[i2], lattice[nearest[i2][j]]);
196
197         dr -= ((lattice[i1] + lattice[nearest[i1][j]]) == 1)
198             + ((lattice[i2] + lattice[nearest[i2][j]]) == 1);
199     }
200     /* Then we do the change of the two atoms */
201     lattice[i1] = old_2;
202     lattice[i2] = old_1;
203     for( int j=0; j<N_neigh; j++){
204         /*
205          And _add_ the contributions to `Etot` and `r` from the updated lattice.
206          */
207         dE += +get_bond_E(lattice[i1], lattice[nearest[i1][j]])
208             + get_bond_E(lattice[i2], lattice[nearest[i2][j]]);
209
210         dr += ((lattice[i1] + lattice[nearest[i1][j]]) == 1)
211             + ((lattice[i2] + lattice[nearest[i2][j]]) == 1);
212     }
213
214     if ( (dE<=0) || (exp(-beta * dE) > gsl_rng_uniform(q)) ){
215         /*
216          The test is accepted if dE < 0 (accept immediately), OR
217          otherwise it's accepted with a probability of `exp(-beta * dE)`
218          */
219         // Updates P
220         if (i1 < N_Cu)
221             *P += (double)(lattice[i1] - old_1 )/N_Cu *2;
222         if (i2 < N_Cu)
223             *P += (double)(lattice[i2] - old_2 )/N_Cu *2;
224     }else{
225         /*
226          If the test failed, we change back to the old lattice configuration
227          and no change happens to `Etot` or `r`
228          */
229         lattice[i1] = old_1;
230         lattice[i2] = old_2;
231         dE = 0;
232         dr = 0;
233     } // end if step is accepted
234     *Etot += dE;
235     *r += dr/(4*N_Cu);
236 } // end if atoms are different
237 }
238
239 void update_E_P_r(int iT, double E_dev, double *E_mean, double *E_sq_mean,
240                 double P, double *P_mean, double *P_sq_mean,
241                 double r, double *r_mean, double *r_sq_mean,
242                 int *lattice, int (*nearest)[N_neigh], int N_Cu){
243     /*
244      Updates the macro parameters `E`, `P`, and `r`, as well as their squares.
245      Runs in every Monte Carlo step during the production run.
246      */
247     E_mean[iT] += E_dev;
248     E_sq_mean[iT] += E_dev * E_dev;
249
250     P_mean[iT] += P;
251     P_sq_mean[iT] += P*P;
252
253     r_mean[iT] += r;
254     r_sq_mean[iT] += r*r;
255 }
256
257 /***** initializing functions *****/
258 double * init_temps( int *nT, double dT_small, double dT_large,
259                     double T_start, double T_end, double T_start_fine,
260                     double T_end_fine){
261     /*
262      Creates an array `T_degC` with the temperatures to loop over in the main
263      function, given the fine temperature step range and the sizes of the
264      temperature steps.
265      */
266     *nT = (int) ((T_end_fine - T_start_fine)/dT_small
267                 + (T_start_fine-T_start + T_end-T_end_fine)/dT_large +1);
268     double *T_degC = malloc(sizeof(double)*nT);
269     T_degC[0] = T_start;
270     for (int iT=1; iT<*nT; iT++){ // loop over all temps
271         if (T_degC[iT-1]>=T_start_fine && T_degC[iT-1]<T_end_fine){
272             T_degC[iT] = T_degC[iT-1] + dT_small;
273         }else{
274             T_degC[iT] = T_degC[iT-1] + dT_large;

```

```

275     }
276 }
277 return T_degC;
278 }
279
280
281 void init_ordered_lattice(int N_atoms, int N_Cu, int *lattice){
282     /*
283      Initialize lattice with Cu atoms (1) in Cu lattice (i=0:N_Cu-1)
284      and Zn (0) in Zn lattice (i=N_Cu:N_atoms-1):
285     */
286     for( int i=0; i<N_Cu; i++){
287         lattice[i] = 1;
288     }
289     for( int i=N_Cu; i<N_atoms; i++){
290         lattice[i] = 0;
291     }
292 }
293
294 void init_random_lattice(int N_atoms, int N_Cu, int *lattice, gsl_rng *q){
295     /*
296      Initialize lattice with Cu and Zn atoms randomly distributed:
297     */
298     for( int i=0; i<N_Cu; i++){
299         lattice[i] = (int)(gsl_rng_uniform(q)+0.5);
300         lattice[i+N_Cu] = 1-lattice[i];
301     }
302 }
303
304
305 void init_nearestneighbor(int Nc, int (*nearest)[N_neigh]){
306     /*
307      Create a matrix `nearest[i][j]` with the index of the `j`th nearest
308      neighbors to site `i`.
309      N.B. Each site has `N_neigh` (8) nearest neighbors.
310     */
311     int i_atom;
312     int N_Cu = Nc*Nc*Nc;
313     for( int i=0; i<Nc; i++){
314         for( int j=0; j<Nc; j++){
315             for( int k=0; k<Nc; k++){
316                 i_atom = k + Nc*j + Nc*Nc*i;
317                 // k i j in one lattice <=> "k-0.5" "i-0.5" "j-0.5" in the other lattice
318                 // use mod to handle periodic boundary conditions
319                 nearest[i_atom][0] = k + Nc*j + Nc*Nc*i + N_Cu;
320                 nearest[i_atom][1] = k + Nc*j + Nc*Nc*((i+1)%Nc) + N_Cu;
321                 nearest[i_atom][2] = k + Nc*((j+1)%Nc) + Nc*Nc*i + N_Cu;
322                 nearest[i_atom][3] = k + Nc*((j+1)%Nc) + Nc*Nc*((i+1)%Nc) + N_Cu;
323                 nearest[i_atom][4] = (k+1)%Nc + Nc*j + Nc*Nc*i + N_Cu;
324                 nearest[i_atom][5] = (k+1)%Nc + Nc*j + Nc*Nc*((i+1)%Nc) + N_Cu;
325                 nearest[i_atom][6] = (k+1)%Nc + Nc*((j+1)%Nc) + Nc*Nc*i + N_Cu;
326                 nearest[i_atom][7] = (k+1)%Nc + Nc*((j+1)%Nc) + Nc*Nc*((i+1)%Nc) + N_Cu;
327
328                 // k i j in one lattice <=> "k+0.5" "i+0.5" "j+0.5" in the other lattice
329                 // use mod to handle periodic boundary conditions
330                 // note that mod([negative])<0 :
331                 i_atom += N_Cu;
332                 nearest[i_atom][0] = k + Nc*j + Nc*Nc*i;
333                 nearest[i_atom][1] = k + Nc*j + Nc*Nc*((i-1+Nc)%Nc)↵
334
335                 nearest[i_atom][2] = k + Nc*((j-1+Nc)%Nc) + Nc*Nc*i;
336                 nearest[i_atom][3] = k + Nc*((j-1+Nc)%Nc) + Nc*Nc*((i-1+Nc)%Nc)↵
337
338                 nearest[i_atom][4] = (k-1+Nc)%Nc + Nc*j + Nc*Nc*i;
339                 nearest[i_atom][5] = (k-1+Nc)%Nc + Nc*j + Nc*Nc*((i-1+Nc)%Nc)↵
340
341                 nearest[i_atom][6] = (k-1+Nc)%Nc + Nc*((j-1+Nc)%Nc) + Nc*Nc*i;
342                 nearest[i_atom][7] = (k-1+Nc)%Nc + Nc*((j-1+Nc)%Nc) + Nc*Nc*((i-1+Nc)%Nc)↵
343
344             }
345         }
346     }
347 }
348
349 gsl_rng* init_random(){
350     /*
351      Initializes a GSL random nubner generator, and returns the pointer.
352     */
353     gsl_rng *q;
354     const gsl_rng_type *rng_T; // static info about rngs
355     gsl_rng_env_setup(); // setup the rngs
356     rng_T = gsl_rng_default; // specify default rng
357     q = gsl_rng_alloc(rng_T); // allocate default rng
358     gsl_rng_set(q,time(NULL)); // Initialize rng
359     return q;
360 }
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```



```

362  /*
363   Writes the energy per bond `E_equilibration`/'N_bonds` and order
364   parameter `P`, at each Monte Carlo step during the equilibration runs.
365  */
366  FILE *file_pointer;
367  char file_name[256];
368  sprintf(file_name, "../data/E_equilibration-T%d.tsv", (int) T_degC);
369  file_pointer = fopen(file_name, "w");
370  for (int i=0; i<N_eq; i++){
371      fprintf(file_pointer, "%.8f\t%.8f \n", E_equilibration[i]/N_bonds, P[i]);
372  }
373  fclose(file_pointer);
374  }
375
376  void write_production(double *T_degC, int nT, double *E_mean_approx,
377                      double *E_mean, double *E_sq_mean,
378                      double *P_mean, double *P_sq_mean,
379                      double *r_mean, double *r_sq_mean){
380
381      /*
382       Writes the macro parameters `E_mean_approx`, `E_mean`, `E_sq_mean`,
383       `P_mean`, `P_sq_mean`, `r_mean`, and `r_sq_mean` for each temperature
384       to file.
385      */
386      FILE *file_pointer;
387      char file_name[256];
388      sprintf(file_name, "../data/E_production.tsv");
389      file_pointer = fopen(file_name, "w");
390      fprintf(file_pointer, "%s T[degC]\t E_approx\t<E-E_approx>\t<(E-E_approx)^2>\t<E-E_approx>\tP\tP^2\n");
391      for (int iT=0; iT<nT; iT++){
392          fprintf(file_pointer, "%.2f\t%.8e\t%.8e\t%.8e\t%.8f\t%.8f\t %.8f\t%.8f \n",
393                  T_degC[iT], E_mean_approx[iT], E_mean[iT], E_sq_mean[iT], P_mean[iT],
394                  P_sq_mean[iT], r_mean[iT], r_sq_mean[iT]);
395      }
396      fclose(file_pointer);
397  }
398
399  void write_stat_inefficiency_to_file(double T_degC, double *phi, double *var_F,
400                                     int N_k, int N_skip){
401
402      /*
403       Writes the auto-correlation `phi` and block varaiances `var_F` for each
404       tested temperature to file.
405      */
406      FILE *file_pointer;
407      char file_name[256];
408      sprintf(file_name, "../data/stat_inefficiency-T%d.tsv", (int) T_degC);
409      file_pointer = fopen(file_name, "w");
410      for (int i=0; i<N_k; i++){
411          fprintf(file_pointer, "%d\t%.8f\t%.8f \n", i*N_skip, phi[i], var_F[i]);
412      }
413      fclose(file_pointer);
414  }

```

B Auxiliary

B.1 Makefile

```

1
2  CC = gcc
3  CFLAGS = -O3 -Wall
4
5  LIBS = -lm -lgsl -lgslcblas
6
7  HEADERS = funcs.h
8  OBJECTS = funcs.o
9
10
11  %.o: %.c $(HEADERS)
12      $(CC) -c -o $@ $< $(CFLAGS)
13
14  all: Task2
15
16
17
18  Task2: $(OBJECTS) main_T2.c
19      $(CC) -o $@ $^ $(CFLAGS) $(LIBS)
20
21  # $(PROGRAMS): $(OBJECTS) main_T1.c
22  #   $(CC) -o $@ $^ $(CFLAGS) $(LIBS)
23
24  clean:
25      rm -f *.o
26      touch *.c

```

C MATLAB scripts

C.1 Task 1 and analysis scripts for Task 2

```
1 %% initial
2
3 tmp = matlab.desktop.editor.getActive; %% cd to current path
4 cd(fileparts(tmp.Filename));
5 set(0,'DefaultFigureWindowState','docked');
6 warning('off','MATLAB:handle_graphics:exceptions:SceneNode'); % interpreter
7 GRAY = 0.7*[0.9 0.9 1];
8 kB = 8.61733e-5;
9 %% task 1: MFT
10 doSave = 1;
11 clc
12
13 Pmin = 0;
14 Pmax = 1;
15
16 E_CuCu = -.436;
17 E_ZnZn = -.113;
18 E_CuZn = -.294;
19
20 E0=2*(E_CuCu+E_ZnZn+2*E_CuZn);
21 Delta_E=(E_CuCu+E_ZnZn-2*E_CuZn);
22 E_max = (E_CuCu + E_ZnZn)/2;
23
24 E0_bar=E0/Delta_E;
25 E_MFT=@(P) E0 - 2*P.^2*Delta_E;
26 E_MFT_bar=@(P) E0_bar - 2*P.^2;
27 dE_MFTdP =@(P) - 4*P*Delta_E;
28
29 F_MFT = @(P,Tbar) E_MFT_bar(P) + Tbar*(-2*log(2) + (1+P).*log(1+P)+(1-P).*log(1-↵
    P));
30 P_eq=@(Tbar) fminbnd(@(P)F_MFT(P, Tbar), Pmin, Pmax, optimset('TolX',1e-9));
31
32 Tbar = linspace(0,3,1000)';
33 T_MFT=Tbar*Delta_E/kB;
34 T_MFT_degC = T_MFT - 273.15;
35 Peq = zeros(size(Tbar));
36 for iT = 1:numel(Tbar)
37     Peq(iT) = P_eq(Tbar(iT));
38 end
39
40 % plot P(T) and make a fit
41 figure(1);clf
42 plot(Tbar, Peq);hold on
43
44 dT=2-Tbar(Tbar<2);
45 Peq_nonzero = Peq(Tbar<2);
46
47 I_good = (dT<0.1);
48 log_dT = log(dT(I_good));
49 log_P = log(Peq_nonzero(I_good));
50 A=[ones(size(log_dT)), log_dT]\log_P;
51 b = exp(A(1));
52 alpha = A(2);
53 fprintf('alpha = %.3f\n', alpha)
54
55 P_approx = @(alpha,b,Tbar) b*(2-Tbar).^alpha;
56 plot(Tbar(Tbar<2),P_approx(alpha,b,Tbar(Tbar<2)),'k:');
57 xlabel('$\bar{T}$')
58 ylabel('$P$')
59 legend('$P$', 'fit $P \propto (2-\bar{T})^\beta$', 'location', '↵
    NorthWest');
60 ylim([0 1.3]);
61 if doSave; setFigureSize(gcf, 300, 600); end
62
63 % plot E_MFT and the fit
64 figure(2);clf
65 plot(Tbar,E_MFT(Peq)); hold on
66 plot(Tbar,E_MFT(P_approx(alpha,b,Tbar)),'k:');
67 xlabel('$\bar{T}$')
68 ylabel('$u$ [eV/cell]')
69 legend('$u_{\rm MFT}$', 'fit $P \propto (2-\bar{T})^\beta$', 'location', '↵
    NorthWest');
70 ylim([-2.36 -2.3]);
71 if doSave; setFigureSize(gcf, 300, 600); end
72
73 figure(3);clf
74 C_MFT=diff(E_MFT(Peq))./diff(T_MFT);
75 plot(Tbar(1:end-1), C_MFT*1e3); hold on
76 C_approx=4*b^2*kB*alpha*(2-Tbar).^(2*alpha-1);
77 plot(Tbar(Tbar<2),1e3*C_approx(Tbar<2),'k:');
78 xlabel('$\bar{T}$')
79 ylabel('$C$ [meV K$^{-1}$]/cell]')
80 legend('$C_{\rm MFT}$', 'fit $P \propto (2-\bar{T})^\beta$', 'location', '↵
    NorthWest');
```

```

81 ylim([0 0.3])
82 if doSave; setFigureSize(gcf, 300, 600); end
83
84 ImproveFigureCompPhys()
85 if doSave
86     saveas(1, '../figures/P_MFT.eps', 'epsc');
87     saveas(2, '../figures/E_MFT.eps', 'epsc');
88     saveas(3, '../figures/C_MFT.eps', 'epsc');
89 end
90
91
92 %% task 2: equilibration and statistical inefficiency
93 clc;
94 doSave = 1;
95 Ts = [-200:20:1000];
96 TsToPlot = [300 440 600];
97 t_eq=0;
98
99 figure(1);clf;
100
101 for i=1:numel(TsToPlot)
102     data = load(sprintf('../data/E_equilibration-T%d.tsv',TsToPlot(i)));
103     E = data(:,1)*8; % convert from energy per bond to energy per cell
104     steps = 1:length(E);
105     plot(steps, E); hold on
106 end
107 legstr = strcat({'$T='}, num2str(TsToPlot), '$\circ$ C');
108 legend(legstr, 'location', 'NorthWest');
109 ylabel('$E$ [eV/cell]')
110 xlabel('$N_{\rm steps}$')
111 ax = gca;
112 ax.XTickLabel = {'0', '$10^5$', '$2\cdot 10^5$', '$3\cdot 10^5$', '$4\cdot 10^5$', '$5\cdot 10^5$'};
113
114 ImproveFigureCompPhys(1)
115
116 figure(3); clf;figure(2); clf;
117 [ns_Phi,ns_block] = deal(nan(size(Ts)));
118 Nskip = 10; % did not use all k's when calculating block averages
119 N_avg = 100; % moving average
120 for i=1:numel(Ts)
121     data = load(sprintf('../data/stat_inefficiency-T%d.tsv',Ts(i)));
122     k = data(:,1);
123     block_size = k+Nskip;
124     phi = data(:,2);
125     VarF_norm = data(:,3);
126     kstar = k(find(log(phi)<=-2, 1, 'first'));
127     if ~isempty(kstar)
128         ns_Phi(i) = kstar;
129     end
130
131     filtereddata = movmean(VarF_norm,N_avg);
132     ns_block(i) = max(filtereddata);
133
134     if any(Ts(i) == TsToPlot)
135         figure(2)
136
137         semilogx(k, log(phi));hold on;
138         plot([0.1 kstar kstar], [-2 -2 -6],':k')
139
140         figure(3)
141         semilogy(block_size, VarF_norm, '.'); hold on;
142         plot(block_size(N_avg:end), filtereddata(N_avg:end));
143         plot(block_size, ns_block(i)*ones(size(block_size)), ':k');
144
145     end
146 end
147
148 figure(4); clf;
149 plot(Ts, ns_Phi, 'k',Ts, ns_block, '--r')
150 ax = gca;
151 ax.YTickLabel = {'0', '$10^5$', '$2\cdot 10^5$', '$3\cdot 10^5$', '$4\cdot 10^5$', '$5\cdot 10^5$'};
152 ylabel('$n_s$');
153 legend('correlation function $\Phi$', 'block average');
154 xlabel('$T$ [$\circ$C]');
155 ImproveFigureCompPhys(gcf)
156
157 legs_Phi = cell(6,1);
158 legs_block = cell(9,1);
159 for i = 1:numel(TsToPlot)
160     tt = ['$T=' num2str(TsToPlot(i)) '$\circ$C: '];
161     legs_Phi{1 + 2*(i-1)} = [tt 'data'];
162     legs_Phi{2 + 2*(i-1)} = 'estimated $n_s$';
163     legs_block{1 + 3*(i-1)} = [tt 'data'];
164     legs_block{2 + 3*(i-1)} = 'moving average';
165     legs_block{3 + 3*(i-1)} = 'estimated $n_s$';
166 end
167
168 figure(2);
169

```

```

170 legend(legs_Phi, 'location', 'northeastoutside');
171 xlabel('$k$'); ylabel('ln $\Phi_k$');
172 ylim([-3.5 0]);
173 xlim([2e3 3e5])
174 figure(3);
175 ax = gca;
176 [ax.Children(:).MarkerSize] = deal(12);
177 legend(legs_block, 'location', 'northeastOutside');
178 xlabel('block size $B$');
179 ylabel('$B$ Var[$F$]/Var[$f$]');
180 ylim([2e3 2e5])
181 ax = gca;
182 ax.XTickLabel = {'0', '$10^5$', '$2\cdot 10^5$', '$3\cdot 10^5$', '$4\cdot 10^5$', '$5\cdot 10^5$'};
183
184 ImproveFigureCompPhys(2, 'LineColor', {'LINNEAGREEN', 'LINNEAGREEN', 'GERIBLUE', 'GERIBLUE', 'k', 'k'}, ...
185 'LineStyle', {':', '-.', ':', '-', ':', '--'})
186 ImproveFigureCompPhys(3, 'LineColor', {'LINNEAGREEN', 'LINNEAGREEN', 'LINNEAGREEN', 'GERIBLUE', 'GERIBLUE', 'GERIBLUE', 'k', 'k', 'k'}, ...
187 'LineStyle', {':', '-.', 'none', ':', '-', 'none', ':', '--', 'none'});
188
189 if doSave
190     figure(1);
191     setFigureSize(gcf, 300, 600);
192     saveas(gcf, '../figures/equilibration.eps', 'eps');
193     figure(2);
194     setFigureSize(gcf, 350, 900);
195     saveas(gcf, '../figures/stat_inefficiency_Phi.eps', 'eps');
196     figure(3);
197     setFigureSize(gcf, 350, 900);
198     saveas(gcf, '../figures/stat_inefficiency_block.eps', 'eps');
199     figure(4);
200     setFigureSize(gcf, 300, 600);
201     saveas(gcf, '../figures/stat_inefficiency_both.eps', 'eps');
202 end
203
204 %% task 2: U, C, P and r
205
206 doSave = 1;
207
208 data = load('../data/E_production.tsv');
209 T_degC = data(:,1);
210 N_Cu = 1e3;
211 N_timeSteps = 1e7;
212
213 Emean_approx = data(:,2)/N_Cu; % divide by N_Cu to get energy and Cv per cell
214 Emean_shifted = data(:,3)/N_Cu;
215 E_sq_mean_shifted = data(:,4)/N_Cu^2;
216
217 E_Var = (E_sq_mean_shifted - Emean_shifted.^2);
218
219 Cv = 1./(kB * (T_degC+273.15).^2).*E_Var*N_Cu;
220 U = (Emean_shifted + Emean_approx);
221 U_std = sqrt(E_Var/N_timeSteps);
222 P = data(:,5);
223 P_std = sqrt((data(:,6)-P.^2)/N_timeSteps); % without ns so far
224 r = data(:,7);
225 r_std = sqrt((data(:,8)-r.^2)/N_timeSteps);
226
227 ind = zeros(size(Ts));
228 for i = 1:numel(Ts)
229     ind(i) = find(Ts(i) == T_degC);
230 end
231
232 figure(1);clf;
233 plot(T_degC, U); hold on;
234 errorbar(Ts, U(ind), 2*U_std(ind).*sqrt(ns_Phi), 'k', 'linewidth', 2.5); hold on
235
236 plot(T_MFT_degC, E_MFT(Peq), '-.'); hold on
237 ImproveFigureCompPhys(gcf, 'LineColor', {'GERIBLUE', 'r'});
238 legend('$u$', '$u_{\pm 2 \sigma}$ (with $n_{s, \rm \Phi}$)', '$E_{\rm MFT}$', 'Location', 'NorthWest');
239 ylabel('$u$ [eV/cell]')
240 axis tight
241
242 figure(2); clf;
243 plot(T_degC(2:end), 1e3*diff(U)./diff(T_degC)); hold on;
244 plot(T_degC, 1e3*Cv);
245 plot(T_MFT_degC(1:end-1), 1e3*C_MFT, '-.');
246 ImproveFigureCompPhys(gcf, 'LineColor', {'GERIBLUE', 'k', GRAY});
247 legend('$C$, {\partial u / \partial T}$', '$C$, {\rm Var}(E)$', '$C_{\rm MFT}$', 'Location', 'NorthWest');
248 ylabel('$C$ [meV/cell]')
249 ylim([0 0.6])
250
251 figure(3);clf;
252 plot(T_degC, P, 'r'); hold on;
253 errorbar(Ts, P(ind), 2*P_std(ind).*sqrt(ns_Phi), 'k', 'linewidth', 2.5); hold on;
254 plot(T_MFT_degC, Peq, '-.k');

```

```

254 ImproveFigureCompPhys(gcf, 'LineColor', {'GERIBLUE', 'r'});
255 legend('$P$', '$P\pm 2 \sigma$ (with $n_{\rm s}, \rm \Phi)$', '$P_{\rm MFT}$', '↔
    Location', 'SouthWest');
256 ylabel('$P$ ')
257 axis tight
258
259 figure(4);clf;
260 plot(T_degC, r, 'r');hold on;
261 errorbar(Ts, r(ind), 2*r_std(ind).*sqrt(ns_Phi), '.k','linewidth', 1.5);hold on;
262 plot(T_degC, P.^2, '--', T_MFT_degC, Peq.^2, '-.');
263 ImproveFigureCompPhys(gcf, 'LineColor', {'GERIBLUE', 'LINNEAGREEN', 'r'});
264 legend('$r$', '$r\pm 2 \sigma$ (with $n_{\rm s}, \rm \Phi)$', '$P^2$', '$r_{\rm MFT}$↔
    ', 'Location', 'SouthWest');
265 ylabel('$r$ ')
266 axis tight
267 ImproveFigureCompPhys((2:4), 'linewidth', 2)
268
269 if doSave
270     for ifig = 1:4;
271         figure(ifig)
272         setFigureSize(gcf, 300, 600);
273         xlabel('$T$ [$^\circ\rm C]$');
274         xlim([-200 1000])
275     end
276     ImproveFigureCompPhys(1:4);
277     saveas(1, '../figures/U.eps', 'eps');
278     saveas(2, '../figures/C.eps', 'eps');
279     saveas(3, '../figures/P.eps', 'eps');
280     saveas(4, '../figures/r.eps', 'eps');
281 end
282
283 %% test with critical exponents
284 Tcrit = 430;
285 dT=Tcrit-T_degC(T_degC<Tcrit);
286 P_nonzero = abs(P(T_degC<Tcrit));
287
288 I_good = (dT<30 & P_nonzero>0.4);
289 log_dT = log(dT(I_good));
290 log_P = log(P_nonzero(I_good));
291 A=[ones(size(log_dT)), log_dT]\log_P;
292 b = exp(A(1));
293 alpha = A(2);
294 fprintf('P: beta = %.3f\n', alpha)
295 P_approx = @(alpha,b,T) b*(Tcrit-T).^alpha;
296
297 %figure(5);clf;
298 %loglog(dT,P_nonzero) ; hold on;
299 %plot(dT, P_approx(alpha, b, Tcrit-dT), 'g')
300
301 figure(3)
302 Tvec = linspace(300,Tcrit);
303 plot(Tvec, P_approx(alpha, b, Tvec), ':k')
304 ImproveFigureCompPhys(gcf)
305
306
307
308 Cv_good = abs(Cv(T_degC<Tcrit));
309 I_good = (dT<150);
310 log_dT = log(dT(I_good));
311 log_C = log(Cv_good(I_good));
312 A=[ones(size(log_dT)), log_dT]\log_C;
313 b = exp(A(1));
314 alpha = A(2);
315 fprintf('Cv: alpha = %.3f\n', alpha)
316 C_approx = @(alpha,b,T) b*(Tcrit-T).^alpha;
317
318 %figure(6);clf;
319 %loglog(dT,Cv_good) ; hold on;
320 %plot(dT, C_approx(alpha, b, Tcrit-dT), 'g')
321
322 figure(2);
323 plot(Tvec, 1e3*C_approx(alpha, b, Tvec), ':r')
324 ImproveFigureCompPhys(gcf)
325 %% test U as a function of r
326 clf;
327 Ufunc = @(r) 4*(r+1)*E_CuZn + 2*(E_ZnZn+ E_CuCU) * (1-r);
328 plot(r, U, 'k',r, Ufunc(r), ':r')
329 ImproveFigureCompPhys(gcf)

```

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 ←
    proper graphics handles
28 nFigs = length(figHs);
29 end
30
31 % Define desired properties
32 titleSize = 24;
33 interpreter = 'latex';
34 lineWidth = 4;
35 axesWidth = 1.5;
36 labelSize = 22;
37 textSize = 20;
38 legTextSize = 18;
39 tickLabelSize = 18;
40 LineColor = {};
41 LineStyle = {};
42 Marker = {};
43
44 % define colors
45 co = [ 0 0.4470 0.7410
46 0.8500 0.3250 0.0980
47 0.9290 0.6940 0.1250
48 0.4940 0.1840 0.5560
49 0.4660 0.6740 0.1880
50 0.3010 0.7450 0.9330
51 0.6350 0.0780 0.1840 ];
52 colors = struct('MYBLUE', co(1,:), ...
53 'MYORANGE', co(2,:), ...
54 'MYYELLOW', co(3,:), ...
55 'MYPURPLE', co(4,:), ...
56 'MYGREEN', co(5,:), ...
57 'MYLIGHTBLUE', co(6,:), ...
58 'MYRED', co(7,:), ...
59 'GERIBLUE', [0.3000 0.1500 0.7500], ...
60 'GERIRED', [1.0000 0.2500 0.1500], ...
61 'GERIYELLOW', [0.9000 0.7500 0.1000], ...
62 'LIGHTGREEN', [0.4 0.85 0.4], ...
63 'LINNEAGREEN', [7 184 4]/255);
64
65 % Loop through the supplied arguments and check for properties to set.
66 for i = 1:nargin
67 if ischar(varargin{i})
68 switch lower(varargin{i}) %Compare lower case strings
69 case 'linewidth'
70 lineWidth = varargin{i+1};
71 case 'linestyle'
72 LineStyle = varargin{i+1};
73 case 'linecolor'
74 LineColor = varargin{i+1};
75 for iLineColor = 1:numel(LineColor)
76 if isfield(colors, LineColor{iLineColor})
77 LineColor{iLineColor} = colors.(LineColor{iLineColor});
78 end
79 end
80 case 'marker'
81 Marker = varargin{i+1};
82 end
83 end
84 end
85 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
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

```

```

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

```