Project 4
Studies of phase transition in magnetic systems

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The motivation of the project, is to explore stochastic modeling of nature. A magnetic phase shift is explored with Metropolis Markov Chain Monte Carlo simulations. The system is simulated for various 2 dimensional lattice sizes over a scaled temperature range. The system is modeled using the Ising method for a ferro magnet, with no assumed external magnetic field. Near the critical temperature, there is an indication of a discontinuity in correlation, but what is likely lacking data leaves a shaky conclusion.

I. INTRODUCTION

The aim here, is to get used to the Monte Carlo simulation of a system and see how it challenges the intuition of the user. With the Ising method to simulate the system, run a comparative test of energies and control these to a probabilistic rule which allows for some dynamicism in the system. As with most things, I started from the bottom with a 2 by 2 lattice and acode meant specifially for this. [1]

II. METHODS AND THEORY

We want to study a 2 dimensional ferromagnetic system through the Ising model, specifically in phase transitions. The system we're studying has an energy

$$E = -J \sum_{<kl>}^{N} s_k \, s_l$$

In which the "$< kl >$" signifies summing over neighbouring spots in the lattice only. $s_k = \pm 1$, and N is the total number of spins in the latice. J is a coupling constant and, as we are currently investigating ferromagnetic elements we have $J > 0$. As we will investigate changes in the system, the equation can be solved as

$$\Delta E = 2Js_l^1 \sum_{<k>}^{N} s_k$$

.

The numerical issues we focus on through the project, is periodic boundary conditions as well as the metropolis algorithm.

As with most systems, we begin with a simple iteration. For the ising model of ferromagnets, we start out with a 2×2 lattice to find as well as the mean average magnetic moment henceforth "mean magnetism". Additional valuable properties are the specific heat capacity, as well as succeptability as functions of T, with periodic boundary conditions.

$$\langle E(T) \rangle \,, \qquad |M(T)|, \qquad C_V(T), \qquad \chi(T)$$

Having studied simple system, we will write a code of the Ising model to analyse it and use our previous results as benchmarks for further expansion. We want to accurately extract the properties found previously, for a scaled temperature $T = 1$ with dimensions $[T] = \frac{J}{kT}$. Here, k is the Boltzman constant. This will allow us to cancel out the k in future calculations. Another important step, is to log the number of Monte Carlo (MC) cycles we run.

mat<double> $Transfer = [e^{-\Delta E/\beta}\ ]$;
for $n = 1$ **to** L^2 **do**
$x_r, y_r = RNG$;
$\Delta E = 2 \cdot s[x_r, y_r] \sum_{\langle k \rangle} s_k$;
$r = RNG_{uniform} \in [0, 1]$;
if $r \leq Transfer(\Delta E)$ **then**
$s[x_r, y_r] * = -1.0$;
$M+ = 2 \cdot s[x_r, y_r]$;
$E+ = \Delta E$;
end
end

Algorithm 1:

Having Benchmarked and controlled our program for a simple system, we up the lattice size $L \times L$ to $L = 20$. To abvoid wasting cpu cycles on usesless info that will at best be thrown out, we need to determine the time the system needs to reach equilibrium. The simplest method here, is to just plot the various expectation values as functions of the number of MC cycles. and determining by-eye when the system reaches the desired stability. Time is measured in sweeps of MC cycles per lattice. An interesting question, is whether or not the equilibration time depends on the starting position. Whether this is ordered so all spins point in the same direction or random configuration. These first tests will be run with the initial temperature $T = 1$. We will also investigate the temperature $T = 2.4$ and whether or not it is possible to estimate equilibration time. Here, we want to plot the total number of accepted MC cycles as a function of the total number of MC cycles run, so as to investigate whether or not we can attest to the accepted configurations depending on T.

Additionally we want to study the probabilities for energies, $\Pr(E)$, in effect counting up the number of times the energy E comes up in the computation. We begin our counting after having reached equilibrium to ensure statistically significant readout. We want the energetic variance σ_E^2.

With our system set up, we can now study the properties of the system as we change the temperature. There is a phase shift of the system on the crossing of a certain critical temperature T_C. Below this, the energy is low enough, so that the bias in energetic preference freezes the system towards the energetic minimum. This should result in growing clusters of spins, untill the system eventually inhabits the minimum energy state where all spins point in the same direction. With temperatures greater than T_C, the energety present lessens the bias towards the energetically preferable state. This means that the clusters of similar spins are smaller and more spread, with a more random distribution.

Near T_C we can characterize several properties of the system with a power law behaviour. In the Ising model, the mean magnetisation is given by

$$\langle M(T)\rangle \sim (T - t_C)^{\beta} \quad \text{with} \quad \beta = \frac{1}{8}$$

Here, β is called the "critical exponent". Similar expressions can be found for heat capacity and susceptibility:

$$C_V(T) \sim |T_C - T|^{\alpha}, \qquad \alpha = 0$$
$$\chi(T) \sim |T_C - T|^{\gamma}, \qquad \gamma = \frac{7}{4}$$

The 0 exponent stems from logarithmic divergence, where the value arises from a rewrite into the Taylor series, where $|T_C - T|^{\alpha} \simeq -\ln(|T_C - T|) + O(\alpha^2)$. This is an exponentially growing "spike" around the critical temperature.

Another important quantity is correlation length, ξ. For temperatures $T \gg T_C$, the correlation between the spins should be so low, that the correlation length should be on the order of the distance between each lattice point. As we approach the critical temperature from above, this correlation length grows with a divergent behaviour

$$\xi(T) \sim |T_C - T|^{-\nu}$$

The 2^{nd} order order correction is characterised by a ξ spanning the system. A finite lattice, therefore has a correlation length proportional to the lattice size. Using so-called "finite size scaling relations" we can relate the behaviour of ξ to the infinite span. With this, the critical temperature scales as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}$$

Where a is some constant and ν is as defined for ξ above. When we set $T = T_C$, the above equations go to:

mean magnetisation:

$$\langle \mathcal{M}(T)\rangle \sim (T - T_C)^{\beta} \to L^{-\beta/\nu}$$

Heat capacity:

$$C_V(T) \sim |T_C - T|^{-\gamma} \to L^{\alpha/\nu}$$

and succeptibility:

$$\chi(T) \sim |T_C - T|^{-\alpha} \to L^{\gamma/\nu}$$

We want to study these numerically relations in our system when it is near T_C. We want to examine the dependence of T and L for the listed characteristics. We also want to time these tests, to compare between parallelization of the code. Finally, we want to compare our critical temperature above to the closed-form solution found by Onsanger in 1944: $kT_C/J = 2/\ln\left(1 + \sqrt{2}\right) \approx 2.269$ [2].

III. RESULTS AND DISCUSSION

With these values to control against, we can now benchmark our program. Writing out a few functions, we have one for setting up our lattice, one for running through an MCcycle and one for writing the results to file. I store the expectation vales of the energy, the energy squared and the same for the magnetization, as well as the absolute value per microstate. These can be used directly, in the case of the energy expectation value and the mean magnetization, or in combination such as with the heat capacity and susceptibility, who's scaled values are the variance in either energy or magnetization expectation values. Both of these values are important in any MC calculation, because they give a sharp definition of the statistical sharpness of the result. we see that they approach the analytical values well after 1e6 cycles, with

The Monte Carlo method is, by nature a stochastic representation, where we simulate the system as it evolves with time. Therefore, We have no guarantee that the state is in it's most likely form. As our statistical models are based on an equilibrium assumption, they do not give accurate results unless we are in a stable position. As a test for this, we run the now benchmarked program over a lattice of $L = 20$ spin states in 2 directions and store the expectation energy and mean magnetization $\langle E\rangle$ and $\langle |M|\rangle$. We can see that for the low temperature, the expectation energy lies at about $-2J$ per sping, J is here the coupling constant between the spin, not Joule. Looking back at the Ising model, we can see that this means more or less every spin points in the same direction. As we increase the temperature, we notice that the resting energy is higher. This makes sense if we consider that there are more energy within the system which allows for some spins to be in less energetically preferential positions.

Another interesting facet, is the probability of each energy for the system durign these states. As we measure statistical values, probability would merely be a scaled frequency of energies. Storing these, we can make a normalized histogram to ilustrate, see fig3 If we look at the histogram in figure 3, I would place the peak probability in 799 and 450 or 475 respectively, based on the height difference observed. According to my computed variance, $\sigma_E^2 =$, we can check the validity of our measurements.

Having observed these changes in the state over the different temperatures, we now want to study the system to see if there is a gradual change, or a more distinct one, akin to the shift from ice to water with tempera-

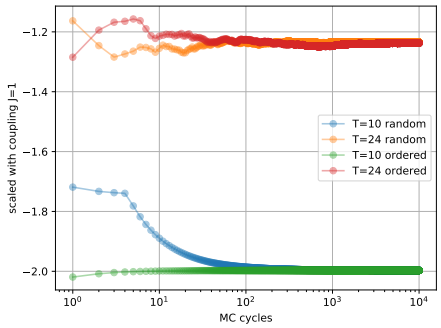

FIG. 1. Plot of $\langle E \rangle$ for a lattice of size $L = 20$ for temperatures $T = \{1.0, 2.4\}$. We can see that there clearly is a difference in the convergence of the different temperatures, with the higher temperatures having a higher average energy. This is as we would expect. We can see, that both graphs seem to have settled towards a stable value somewhere in between 10^2 and 10^3 cycles through the lattice. What is not obvious, is that the numbers displayed are only $\frac{1}{100}$ of the actual values, as I failed to specify an x-axis, yet plotted every 100th element. this brings the Equilibration time closer to 10^4, which is what I've used for the remainder of the project.

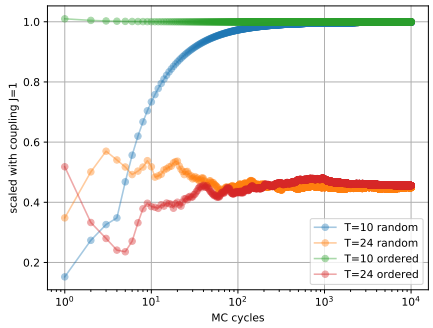

FIG. 2. we can see that the magnetization approaches 1 for the lower temperature. as it is scaled in our model, this means that efectively all spins point in the same direction. as we increase the temperature, and the spins can change a bit more freely, we get a lower magnetization. there is increased turbulence for the higher temperature, but i would say we have reached a mostly stable state at around 10^2 or slightly above, as with the energy. this is in agreement with fig **??**.

ture. As my model was not object oriented, The changes required were somewhat extensive. The result was a second, eventually third, iteration of my Monte Carlo simulation, "MCCycleLarge". With the setup, I attempted to remove as much as possible from the various loops. The result was discarding the previously stored values in favour of an "ExpectationValues" array accumulating data through the sweeps. I also split each set of cycles in 2 loops. The first was to equilibrise the system without storing any data. The split was motivated by a desire to avoid if-tests. These are in a function which I call within

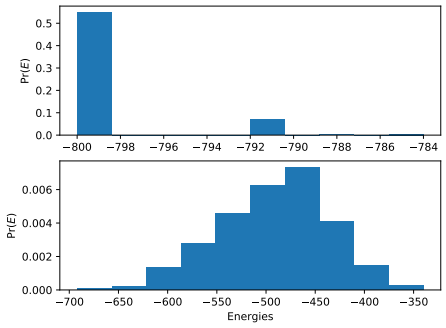

FIG. 3. A scaled histogram of the occurences of various energies of the lattice over time. The upmost one is of a temperature $T = 1.0$ and the lower has $T = 2.4$. As one would expect, without energy in the system, there is very little the particles in the lattice can do to not follow the energetically advantageous configuration. We can also notice, that between the 2 largest columns, there is a gap of $8J$, which is the energy from 4 ordered to 1 disordered spin state, which follows our model. There is another slight bump with $8J$ less energy as well. The lower of the 2 is for the more energetic $T = 2.4$ state. Here we see a far greater spread of energies, this time there are fewer configurations where all spins point in the same direciton, but the vast majority of the states are in above the -400 energy state, which would be half of the low-energy state. The shape is somewhat reminiscent of the Boltzmann distribution of states.

a nested loop of the ranges of temperature and lattice size. Sweeping over lattices $L = \{40, 60, 80, 100\}$, and temperatures $T \in \{2.2, 2.3\}$ with a step of $\Delta T = 0.01$, using a foreknowledge of Onsanger's results at $T_C = 2.27$, to shrink the range, while keeping some precision. I did not quite have the time to parallellize the code, so I saw it as a necessary sacrifice. After leaving the program to slow cook overnight, I could finally start to process the results.

Ideally, following the idea of a phase shift, we should see some sort of extrema in this range. The $\langle E \rangle$ is mostly linear throughout the range, and the susceptibility spreads out far toom much for me to give any indications as to the magnetic change of state. For the latter 2, there is some change, however. The range around 2.27 seems to be the temperatures at which the mean magnetization begins to plummet, indicating a far less cohesive spin direction after this rough value, where there would likely be little coherence in spin direction across the lattice. The heat capacity too, has a peak in this rough area.

IV. CONCLUSION

There seems to be indications of a phase shift in this area, as we can see the system behaviour differing over the temperatures, but the "peak" in heat capacity is not very pronounced, and is not a reliable proof here. If

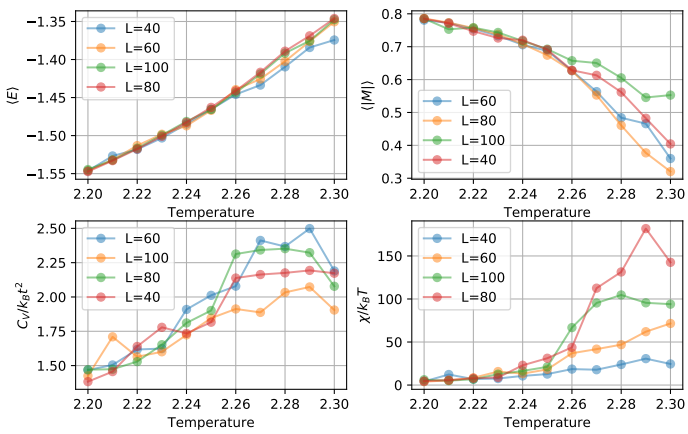

FIG. 4. The figure above is the mean energy, $\langle E \rangle$, the mean magnetization, $\langle |M| \rangle$, the heat capacity a constant volume, C_V scaled by $k_B \cdot T^2$ for simplicity during calculation, effectively the energetic variance per spin, and the susceptibility χ scaled by $k_B \cdot T$ to the effect of taking the variance of the absolute magnetization of the system. Following Onsanger's prediction, we should expect to see a critical temperature at around the temperature 2.27. The mean energy per particle seems to increase fairly linearly with temperature, but the magnetization drops of towards 0, in what seems to be an exponential trend, with the full decent beginning in between 2.26 and 2.28. I can also see the beginning of an extremum in the range 2.26 to 2.30 for the heat capacity of the system, seeming to suggest that this is the range where the greatest amount of energy is required to change the temperature. This too is to be expected in a phase shift. There could possibly be a spike in the susceptibility in this range as well, but the different lattice sizes produce so widely differing results here, that I am loathe to give a definitive suggestion.

there was indeed a phase shift, then I would expect to see a fairly high difference in the energies of some particles with regards to others. I take ice melting as an example here. During the process of melting, som molecules would be frosen while others would be free to move about. After having melted, all particles are equally as free to move. Similarly, if before the phase shift, the molecules were kept in place by the energy needed to supplant the energetically prefreable configuration, then around the area where they could "break free", I would expect to see a more sporadic shift in areas, leading to a far greater spred from the mean. This should lead to quite a spike in the heat capacity, which I simply don't see. I expect this fact comes from a lack of data. The stochastic nature of the Monte Carlo methods demand a great deal of points. Points which I was unable to provide. If I had been able to scrounge up the time to parallellize the code I believe I could have reproduced a far stronger peak, as well less drift between the lattice sizes.

While the code gave the correct energies for given configurations of the lattice, as well as converged towards the correct analytical values for the closed form 2 by 2 solution, If I initialized the lattice in a random position, the resulting convergence was towards a number more negative than $-2J$ per particle, something is unphysical. I do not know if this is a fault in the code, the model or my implementation of it. It is, nonetheless, important to bring up, should a problem arise.

Another point of research which could be usefull, is the state where all spins are flipped. In this instance, the energy wouldn't change, and thus it should posess no suppression from the model, and yet I believe this is a very unlikely event given the decoupling of the spins with their further neighbours. I do not know much about it, but I believe that for a system with no external force a so called "wolf cluster" [3].

The project has some glaring flaws, in that it is neither object oriented, nor is it parallellized. The object orientation would have helped in both making adjusting the code easy, as well as making the switching between tasks easier. for instance, when going from benchmarking and establishing a general behaviour of the system, to measuring probabilities and eventually to running a larger scale simulation over multiple variables, I was eventually forced to simply copy the program and modify it, rather than potentially losing methods to reproduce earlier results should an error occur. With a system in place to catch, e.g. differing variables to store, I could perhaps tweak the various classes while keeping the overal structure unchanged.

Not having a parallellized code also proved difficult in that even leaving the computation runing over a near 10 hour period, the results were rather poor, with no particular spikes in any variables. Comparing with other run results known to reach MC cycles of up to near 10^9, it is quite understanding that my measly 10^4 per temperature and lattice size can hardly compare.

[1] M. H. Jensen, "Isingmodel.cpp," https://github.com/CompPhysics/Computational-Physics/blob/master/doc/Programs/Parallelization-MPI/IsingModel.cpp.

[2] L. Onsager, Phys. Rev. **65**, 117 (1944).

[3] U. Wolff, Physical Review Letters **62**, 361 (1989).