Critical exponents of 2D Ising model using Swendsen-Wang algorithm

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In this report the 2D Ising model is simulated by a Monte Carlo simulation using the Swendsen-Wang method. Using this simulation the magnetisation (m), magnetic susceptibility (χ) and specific heat (c_v) are determined. These quantities are evaluated around the critical temperature to extract the critical exponents (CE). m behaves as expected with a CE of $\beta = 0.112(2)$. χ on the other hand deviates from the theoretical expectation as it has two different CEs for $(T - T_c) < 0$ and $(T - T_c) > 0$ which are each about 0.4 off from the theoretical value of $\gamma = 1.75$. The theoretical relation for c_v does hold, but only for a temperature range much smaller than for the other quantities. The observations done by χ and c_v are probably due to finite scaling effects but need to be investigated further. The dynamical CE is found to be $z_\chi = 0.19(4)$ which agrees with the literature value of $z_\chi = 0.20(2)$. The simulation run time scales quadratic with system size and linear with the number of time steps.

1. Introduction

The 2D Ising model was the first model found to exhibit a genuine phase transition and was solved exactly by Onsager (1944). As the model prescribes no dynamical evolution it can only be simulated using a Monte Carlo algorithm. First the Metropolis algorithm is implemented after which the final results are generated using the Swendsen-Wang (SW) method. The physics of interest of the 2D Ising model occurs near its phase transition and the Metropolis algorithm slows down drastically near this transition. The SW method does not suffer from this drawback. The phase transition is described by using critical exponents. These will be determined and compared to theoretical values in this report. At the end, simulation performance is discussed of the two algorithms. This report is part of the Computational Physics course (AP3082D) of the Delft University of Technology.

2. Theory

2.1 Ising Model

The Ising model describes the interaction between neighbouring spins within a lattice with Hamiltonian H:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i \tag{1}$$

in which J is the spin coupling constant, $s_i \in \{-1, +1\}$ is the spin at location i, $\sum_{\langle i,j \rangle}$ is the summation over the nearest neighbours j with respect to location i, and h is the strength of the external magnetic field. In 1924-1925 E. Ising found the solution to this problem for a 1D lattice (*'einfache lineare Kette'*). (Ising (1925)) The solution to the 2D Ising model for a zero magnetic field was found by L. Onsager. He saw that there was a phase transition present characterised by the vanishing of the magnetisation of the system. (Onsager (1944))

2.2 Phase transitions

The 2D Ising model has a second order phase transition from a magnetic (ordered) phase to a nonmagnetic (disordered) phase for which the average magnetisation is nonzero and zero, respectively. The presence of this second order phase transition is mathematically shown by Onsager (1944) and visualised in chapter 7.2.2 of Thijssen (2007). The point at which this transition occurs is the so-called critical temperature T_c. For an *infinite* 2D lattice this is given by:

$$\sinh(2J\beta_c)\sinh(2J'\beta_c) = 1 \tag{2}$$

in which $\beta_c = (k_B T_c)^{-1}$, and J, J' are the coupling constants in the two perpendicular directions within the 2D system. (Onsager (1944)) In this report $J' = J$ which results in $(\beta_c J)^{-1} \approx 2.269$.

Critical exponents. In the neighbourhood of the critical temperature the thermodynamic quantities show a behaviour which can be described by so-called critical exponents. The exact solution of the 2D Ising model has the critical exponents shown in table 1. The critical exponent of the specific heat c_v is zero which denotes a logarithmic divergence, namely $c_v \propto \ln|T - T_c|$.

Table 1
Thermodynamic quantities (TDQ) and there relation to the (critical) temperature $T_{(c)}$. Specific heat (c_v), magnetisation (m), magnetic susceptibility (χ) and correlation length (ξ)

Relations of TDQ	Critical exponent
$c_v(T) \propto \lvert T - T_c\rvert^{-\alpha}$	$\alpha = 0$
$m(T) \propto (T_c - T)^\beta$, $T < T_c$	$\beta = 1/8$
$\chi(T) \propto \lvert T - T_c\rvert^{-\gamma}$	$\gamma = 7/4$
$\xi(T) \propto \lvert T - T_c\rvert^{-\nu}$	$\nu = 1$

3. Method

The 2D Ising model is analysed by simulating its behaviour for a square ($N \times N$) lattice with N^2 lattice sites. Each of these lattice sites has a spin with a set value (up or down) when the simulation starts. In order to mimic the infinite 2D lattice, periodic boundaries are applied.

3.1 Monte Carlo simulation

Simulation of the 2D Ising model for a finite grid can be done relatively fast with a Monte Carlo (MC) simulation that uses the aid of Markov chains (MCMC), which is a way of importance sampling. MC simulations require new system configurations for every calculation step (MC step). These configurations can be generated randomly and accepted with a certain probability. However, this may lead to creating unnecessary many configurations that will be rejected and therefor it is not very efficient. In a Markov chains each configuration is generated with a probability distribution depending on the previous configuration, which improves the efficiency. This is characterised by the transmission probability $T(X \rightarrow X')$ which indicates the probability to go from configuration X to X'. In order to give correct results the MCMC has to satisfy the detailed balance equation:

$$\frac{T(X \rightarrow X')}{T(X' \rightarrow X)} = \frac{\rho(X', t)}{\rho(X, t)} \tag{3}$$

in which $\rho(X, t)$ is is the probability of finding the system in state X at time t. (Thijssen (2007))

3.2 Metropolis algorithm

The Metropolis algorithm is a possible MCMC method which consists of generating ergodic Markov Chains. For the case of the 2D Ising model the Metropolis algorithm has the following steps described by Thijssen (2007):

1. A random spin in the 2D grip is selected at location (x, y) and flipped with respect to its original orientation $(X \rightarrow X')$.
2. The energy difference $\Delta E(X \rightarrow X')$ between the initial situation, before the flip of the spin, and the current situation is evaluated. In this energy calculation only the interactions between the neighbouring spin sites of the flipped spin are considered. In the case of a square lattice there are four neighbours.
3. If $\Delta E(X \rightarrow X') < 0$, the new state X' is accepted
4. If $\Delta E(X \rightarrow X') > 0$, the new state X' is accepted with probability $P(X \rightarrow X') = e^{\beta \Delta E(X \rightarrow X')}$.

This procedure satisfies the detailed balance equation (eq. 3) and therefor provides good results as long as the temperature is far from the critical temperature. Once the temperature gets close to the critical temperature, the calculation time increases drastically due to a rapid increase of the correlation time, making this algorithm only applicable in the regime $|T - T_c| \gg 1$. This can also be seen by looking at the expression for the correlation time:

$$\tau = \xi^z \tag{4}$$

combined with the expression for the correlation length ξ from table 1 and the knowledge that the dynamic critical exponent $z_E \approx 2.125$ (Tang & Landau (1987)) shows that the correlation time diverges rapidly in the neighbourhood of the transition point. The subscript of z indicates from what system quantity the dynamic exponent is determined.

3.3 Swendsen-Wang method

Swendsen and Wang came up with a different algorithm in 1987 which is based on spin clusters instead of individual spins. In contrast to the Metropolis algorithm, the Swendsen-Wang (SW) method does not scan the spin sites but the bonds in the Ising lattice in lexicographic order. These bonds connect two neighbouring spins and represent the interaction between the spins. The bonds can be deleted (no interaction) or frozen (infinitely strong interaction). The general procedure is described by Thijssen (2007) as follows:

1. Evaluate all bonds within the Ising lattice and assign zero (deletion) or infinity (freezing) to the bond.
   (a) The two neighbouring spins have opposite orientation $\Longrightarrow$ the bond between the spins is deleted.
   (b) The two neighbouring spins have the same orientation $\Longrightarrow$ the bond between the spins can be deleted with probability $p_d = e^{-2\beta J}$ or frozen with probability $1 - p_d$.

   Result of the bond evaluation is that the lattice is split up in a set of disjoint clusters. Within these clusters all spins are equal.
2. Identify each cluster by using the backtracking routine explained by Thijssen (2007).
3. Assign at random a new spin value, up or down, to each cluster.
4. Perform the next iteration by starting at 1. again.

This method satisfies the detailed balance equation (eq. 3) and, in contrast to the Metropolis algorithm, the dynamic critical exponent z for the SW method is much smaller, namely $z_E \approx 0.35$, found by Swendsen & Wang (1987), or $z_\chi \approx 0.2$ found by Wolff (1989). Which makes clear that z depends on the physical quantity from which it is measured. Thus, compared to the Metropolis algorithm, the SW method makes efficiënt numerical analysis near the phase transition possible.

3.4 Specific heat

The fluctuations of the energy of the system are used to calculate the specific heat of the system. The specific heat per spin (c_v) is given by:

$$c_v = \frac{k_B\beta^2}{N}\left(\langle E^2\rangle - \langle E\rangle^2\right) \tag{5}$$

in which N is the total number of spins within the system, $\beta = (k_BT)^{-1}$, E the total system energy and the brackets denote an time average. (Wimmer (2018)) The results for system size $L = 20$ will be quantitatively compared to figure 10.1 from Thijssen (2007).

3.5 Magnetisation

The average magnetisation per spin of the 2D Ising lattice ($\langle m\rangle$) is a measure to see how well aligned the spins in the system are. When $|\langle m\rangle| = 1$ the spins within the system are all aligned in the same direction. If $|\langle m\rangle| \approx 0$, the spins are ordered quite randomly. The average magnetisation per spin of the system is determined by:

$$\langle m\rangle = \frac{1}{N}\left\langle \sum_i s_i \right\rangle \tag{6}$$

in which s_i is the spin at location i. (Wimmer (2018)) Since the Swendsen-Wang algorithm randomly assigns spin to clusters, the magnetisation oscillates between 1 and -1 when one clusters dominates. To overcome that this averages to zero the squared magnetisation will be looked at. It is expected that for large system sizes the solution converges to a step like function in the theoretical limit of $L \to \infty$. (Thijssen (2007)) Which means $\langle m^2\rangle = 1$ below the critical temperature and $\langle m^2\rangle = 0$ above.

3.6 Magnetic susceptibility

The magnetic susceptibility (χ) is a measure of magnetic properties of a material. It indicates whether a material is attracted to or repelled by a magnetic field. When $\chi < 0$ it is paramagnetic (attracted) and when $\chi > 0$ it is diamagnetic (repelled). The magnetic susceptibility per spin is given by Wimmer (2018):

$$\chi = \beta N\left(\langle m^2\rangle - \langle m\rangle^2\right) \tag{7}$$

Since the magnetic susceptibility over temperature is a measure of the change of magnetisation over temperature, a sharp peak is expected at the critical temperature due to the sudden change of the magnetisation at the phase transition. In the limit of $L \to \infty$ the amplitude of the peak would go to infinity as well. Far from the the critical temperature the magnetic susceptibility is expected to be zero.

3.7 Bootstrapping

The averages in equations 5, 6 and 7 are determined by the bootstrapping technique. For a given data set $\{d_{MC}\}$ of the MC simulations consisting of K data points, the bootstrapping technique randomly picks K data points from this set. From these randomly picked K data points the quantity Q is calculated in the same manner as it would have been calculated from the original data set. This process is repeated n times for the same data set $\{d_{MC}\}$. The n different values of Q are then used to determine the average and the standard deviation of Q.

3.8 Critical exponents

The critical exponents corresponding to the quantities mentioned before are determined by fitting a trial function to the simulated data (c_v, m, χ). The trail function for m and χ is given by:

$$f_{trial} = a|\tilde{T}|^b \tag{8}$$

in which $\tilde{T} = T - T_c$ and a, b are the fit parameters. In case of the magnetisation m, $|\tilde{T}|$ is replaced by ($\tilde{T}$). The specific heat is fitted to:

$$f_{trial} = a\ln|\tilde{T}| \tag{9}$$

The dynamic critical exponent z can be extracted from the peak position of a quantity. In general the peak position scales as $T_{peak} \propto L^{-z}$. (Thijssen (2007)) Hence, data for multiple system sizes is needed. This simulated data is fitted to the following trial function:

$$f_{trial,\,z} = L^{-a} + c \tag{10}$$

The quantity chosen to determine z from is the magnetic susceptibility χ, since this data shows clearly defined peaks. The determined dynamic critical exponent will be compared to $z_\chi = 0.20(2)$ found by Wolff (1989).

4. Results and Discussion

The results presented in this section are for a 2D Ising lattice of sides $L = 40$ unless specifically stated otherwise. The temperature interval chosen starts from $k_BT/J = 3.5$ going down to $k_BT/J = 1.5$ in 80 equidistant steps. Simulations start with all spins in the up position. At every temperature the simulation runs for 5100 MC steps of which the last 5000 MC steps are used to determine the quantities. The first 100 MC steps are needed for the system to adapt to the new temperature. Furthermore, uncertainties are calculated using the bootstrap method with $n = 1000$.

4.1 Specific heat

The specific heat in the system is visualised in figure 1 for several system sizes ($L \times L$) and calculated according to eq. 5. Quantitatively the result for $L = 20$ agrees with

what was found by Thijssen (2007), with a peak at the same height. As expected the peak in the spectrum becomes less flattened when the system size increases and will eventually reach the relation stated in table 1 near the critical temperature. It can also be seen that the location of the peak shifts to lower temperatures when L increases and will eventually go asymptotically to the theoretical $k_B T_c/J \approx 2.269$ for $L \to \infty$.

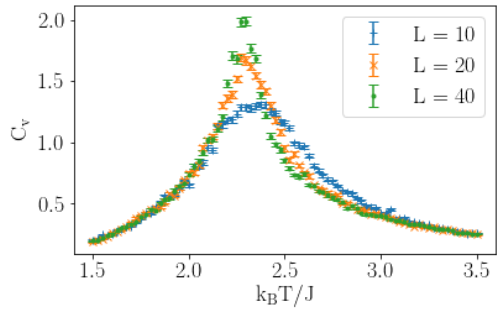

Figure 1. Specific heat near the critical temperature for three system sizes.

4.2 Magnetisation

The magnetisation is calculated according to eq. 6. The behaviour is as expected and seems to converge to a step like function for the limit $L \to \infty$.

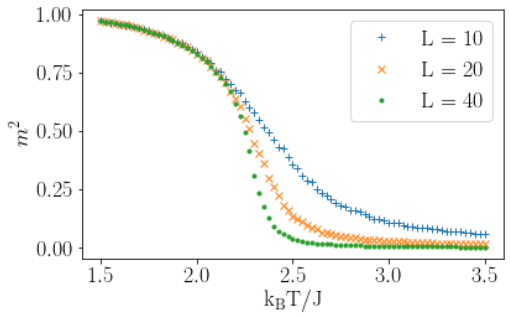

Figure 2. Averaged squared magnetisation near the critical temperature for different system sizes. Varying from $L = 10$ up to $L = 40$. Error bars are omitted as $\sigma < 1\%$.

4.3 Magnetic susceptibility

The results for the magnetic susceptibility are shown in figure 3 and determined according to eq. 7. As can be seen in the figure, the peak within the spectrum becomes more apparent for larger system sizes and also shifts to lower temperatures. In the theoretical limit of $L \to \infty$ the peak will be located at the critical temperature. This is as expected since it should behave as the variance of the magnetisation.

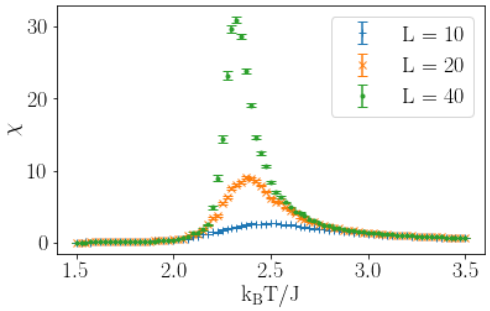

Figure 3. The magnetic susceptibility near the critical temperature for different system sizes.

4.4 Critical Temperature

The critical temperature is determined from the χ peak at $L = 40$, because this has a more distinctive peak than the specific heat. From figure 3 is follows that $k_B T_c/J = 2.30$. The uncertainty in T_c is fully determined by the temperature resolution which is 0.025.

4.5 Critical exponents

Dynamic exponent. To acquire data for multiple system sizes, L is varied from 10 to 40 in steps of 5. This is done for 2100 MC steps in stead of 5100 to save on computation time. Fitting to eq. 10 results for the SW algorithm in $z_\chi = 0.19(4)$, which agrees with the $z_\chi = 0.20(2)$ found by Wolff (1989). The fit is shown in figure 4.

It was also tried to compute this quantity for the metropolis algorithm, but the errors were as big as the quantity itself. This could likely be overcome when the length of the simulation is increased further. Unfortunately, due to time considerations, this was not a feasible option.

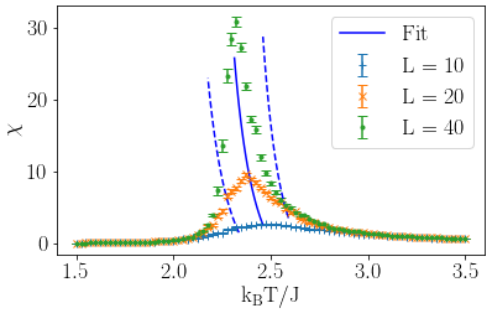

Figure 4. Fit acquired from full L-range ($10 - 40$, $\Delta L = 5$). Three system sizes are plotted to show overall behaviour. The dotted blue lines represent the error in the fit.

Physical quantities. The critical exponents for the magnetisation and the magnetic susceptibility are determined by fitting the trial function (eq. 8) to the acquired data. The trial function is defined with respect to $T - T_c$ while the simulated data is defined with respect to T (the factor k_B/J is omitted for convenience in this section). Therefor the temperature axis needs to be translated with $T_c = 2.3$, which results in an axis with both $(T - T_c) > 0$ and $(T - T_c) < 0$. As the fitting is done in the logarithmic space, the absolute value needs to be taken. (In case of c_v and χ, the theoretical relation is also with respect to the absolute values.) In figure 5 the fit for χ is shown in which the part for $(T - T_c) > 0$ is plotted in blue and $(T - T_c) < 0$ in red.

The fit domain is determined in such a way that the finite size effects are minimised. This is done by excluding the region $|T - T_c| \lessapprox 0.1$. To ensure that the fit is only done in the proximity of T_c, $|T - T_c| < 0.6$ is maintained. As an example, the fit to the magnetic susceptibility is shown.

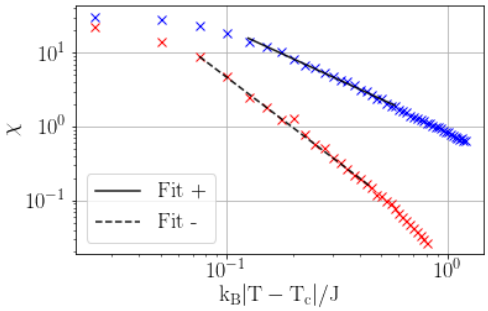

Figure 5. Logarithmic plot of χ including fit. For $(T - T_c) > 0$, χ is in blue with accompanying fit 'Fit +' and for $(T - T_c) < 0$ in red with 'Fit -'.

From figure 5, several observations can be made. First, the flattening of the curve for $|T - T_c|$ close to 0. Secondly, different slopes of the curve for $(T - T_c) < 0$ and $(T - T_c) > 0$. It is believed that both phenomena are due to the finite dimensions of the system. The magnetisation gave no abnormalities and is therefor not graphically shown. Its determined critical exponent is shown in table 2 together with the critical exponents of χ.

Table 2
The critical exponents for m and χ for both temperature domains including the standard deviations

	$(T - T_c) < 0$	$(T - T_c) > 0$
m	$\beta = 0.112(2)$	–
χ	$\gamma = 2.27(3)$	$\gamma = 1.37(2)$

Comparing the exponents from table 2 to the theoretical values in the limit of $L \to \infty$, one sees β is in agreement with the theoretical value. This is not the case for γ as the theoretical value lays between the two found exponents with a relative difference of about 0.4 to both. As said before it is thought that this is due to the finite dimensions of the simulated system.

The trial function for c_v (eq. 9) is fitted to the data, which is shown in figure 6. It is clearly seen that for $|T - T_c| > 0.3$ the positive and negative $(T - T_c)$ domain deviate. Therefor, the fit is adjusted to the region $|T - T_c| < 0.3$ in which c_v behaves logarithmic. Outside this region, the relation from eq. 9 only holds for the negative domain. The origin of this 'odd' behaviour of the specific heat is also thought to be caused by the finite size of the system but needs more investigation.

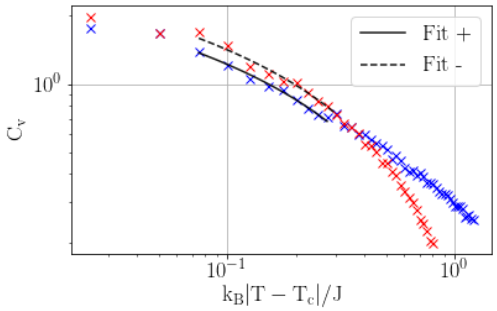

Figure 6. Logarithmic plot of c_v including fit. For $(T - T_c) > 0$, c_v is in blue with accompanying fit 'Fit +' and for $(T - T_c) < 0$ in red with 'Fit -'.

4.6 Code correctness checks

The code is validated in a few ways. First, it is checked if the determined energy of all spins pointing in the same direction (low k_BT/J) corresponds to $-2JL^2$. (Thijssen (2007)) For $L = 20$ and $J = 1$ this is indeed found to be -800 as can be seen in figure 7.

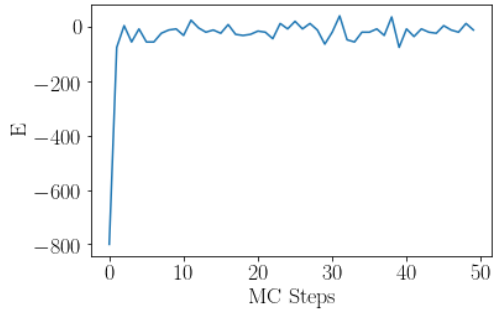

Figure 7. Behaviour of the energy. All spins start in the up position and develop over 50 MC steps for $k_BT/J = 50$.

Second, the overall behaviour of the absolute magnetisation is checked if it indeed goes 1 for low k_BT/J and to 0 for high k_BT/J. This is indeed what happens as can be seen in figure 2. Also behaviour of c_v and χ agrees with literature.

Last, in the Swendsen-Wang algorithm the cluster identification is checked. One such result is shown in figure 8.

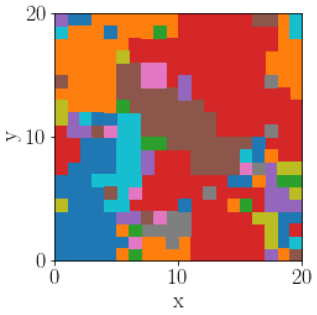

Figure 8. Result of the cluster identification by the backtracking routine for $L = 20$ and $k_BT/J = 2.6$.

4.7 Software performance

Fitting to normalised simulation time we learn that both algorithms scale quadratic in system size. The result is shown in figure 9. SW seems in general almost twice as fast. Their scaling indicates that both algorithms are implement efficiently and that the overhead in calculating quantities is small since both scan the whole lattice to complete a MC step.

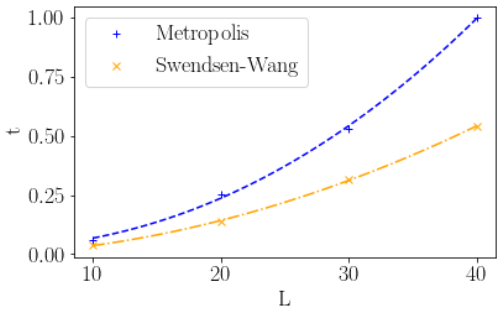

Figure 9. Normalised run time t with respect to system size ($L \times L$) for both Metropolis and Swendsen Wang algorithm.

This view on the simulation performance is still omitting the fact that the SW algorithm has a much smaller dynamical critical exponent. This means that the simulation can be run for a shorter time period to determine the physical quantities and thus makes the SW algorithm much more efficient. Both are linear in MC steps.

To improve performance of the SW algorithm the Hoshen and Kopelman routine can be implemented to identify clusters, which scales linear with system size. (Hoshen & Kopelman (1976)) More advanced algorithms, like the Wolff algorithm, could be implemented to improve efficiency further. However, in case of the Wolff algorithm the improvement is minimal for the 2D Ising model. (Thijssen (2007))

5. Conclusion

From the results presented in this report it can be concluded that the simulation shows appropriate behaviour when the system size increases, as all the physical quantities seem to converge towards the infinite system limit. The determined critical exponent for the magnetisation is in good agreement with the theoretical value for the infinite system size limit. The critical exponents for the other physical quantities show deviations from the infinite system limit, but this is most likely caused by the finite dimensions of the system and the bit arbitrary fitting region. Further simulation for larger system sizes need to be done in order to confirm the suspicion regarding the system size. The fitting region was purely based on visual aid and no firm theoretical background. More knowledge about the needed statistical methods is needed in order to provide this theoretical background. The dynamical critical exponent is determined in agreement with literature.

6. Reflection on cooperation

Like last time cooperation went well. In general the work was split as equal as possible. We started of both working on the metropolis algorithm, where we were developing different parts, but in very close cooperation. For this we also made an animation script to check our results. Then we moved on the to the Swendsen-Wang algorithm and started to use the issue feature like we learned from the first project. We divided the SW algorithm in its main functions and divided them between us as can be seen below. Difficulties during this project were all effectively resolved together or with the help of one of the course instructors. Something to take in mind during the next project is that although there might be an exam week (or other high workload period) it is beneficial to continue developing during this week/period. Now all progress made had to be re-evaluated, because most of it was forgotten. During the entire project results were discussed and code was checked by each other. To give an overview of the specific distribution:

Together: Metropolis, main parts of Swendsen-Wang, spin grid animation
Tom: Data processing to determine critical exponents of magnetisation, magnetic susceptibility and specific heat. Neighbour bond evaluation used in SW.
Vincent: Data acquisition concerning magnetisation, magnetic susceptibility and specific heat. Critical dynamical exponent. Backtracking routine used in SW.

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