Monte Carlo Swendsen-Wang method for 2D Ising Lattice

V.W.J. Heusinkveld (4390725)
Delft University of Technology

T.W.H. de Krom (4281594)
Delft University of Technology

In this paper the 2D Ising model is simulated using a Monte Carlo simulation implement in the form of the Swendsen-Wang algorithm. Using this simulation certain physical quantities are determined. These quantities are looked at around the critical temperature to extract the critical exponent. IN PROGRESS: The behaviour of the magnetisation, magnetic susceptibility and specific heat are all as expected. The found critical exponents are $\beta = TBD$, $\gamma = TBD$ and $\alpha = -0.5$. Where α disagrees with the literature value of 0. This is probably due to a finite scaling effect but needs to be investigated further. The dynamical critical exponent $z_\chi = 0.19(4)$ 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.

Introduction

In the course Computational Physics (AP3082D) several physical problems need to be solved using computational methods. The second problem in the series is the modelling of the magnetic properties of a 2D lattice with spin up or down at every lattice site. A simple model for this is the Ising model combined with a certain Monte Carlo algorithm. In this report, the Ising model will be solved numerically for a 2D lattice by applying two different Monte Carlo algorithms, namely the Metropolis algorithm and Swendsen-Wang method. The Swendsen-Wang method is chosen for determinaton of the results since its performance near the phase transition of the system is much better. In this way we are able to look at the critical exponents and can compare them to exact theoretical values. In the end performance between the two algorithms is discussed.

Theory

Ising Model

The Ising model is a model which describes the interaction between neighbouring spins within a lattice. The model is given by 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, the sum over $\langle i, j \rangle$ is the summation over the nearest neighbours with respect to location i, and h is the magnitude 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))

Phase transitions

The 2D Ising model has a second order phase transition from the magnetic (ordered) phase to the nonmagnetic (disordered) phase. In these phases 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 and J' are the coupling constants in the two perpendicular directions within the 2D system. (Onsager (1944)) The analysis in this report uses $J' = J$ 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
The relevant thermodynamic quantities (TDQ) and there relation to the (critical) temperature $T_{(c)}$. c_v is the specific heat, m is the magnetisation, χ is the magnetic susceptibility and ξ is the correlation length.

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

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.

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))

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.

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.

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).

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.

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.

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.

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 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 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:

$$f_{trial,\,z} = L^{-a} + c \tag{9}$$

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).

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 and run for 5100 MC steps per temperature step. After one run has been completed the temperature is changed and the system gets 100 MC steps to adapt. Hence, the physical quantities are determined using 5000 MC steps of data per temperature step. Furthermore, uncertainties are calculated using the bootstrap method with $n = 1000$.

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 $L \to \infty$.

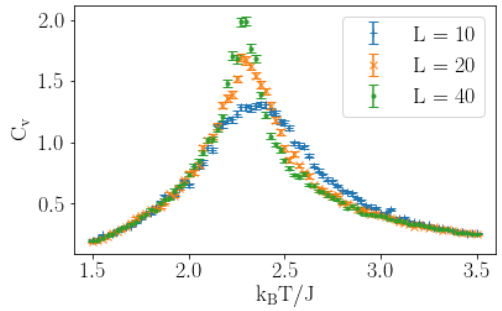

Figure 1. Specific heat near the critical temperature for three system sizes.

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 $L \to \infty$.

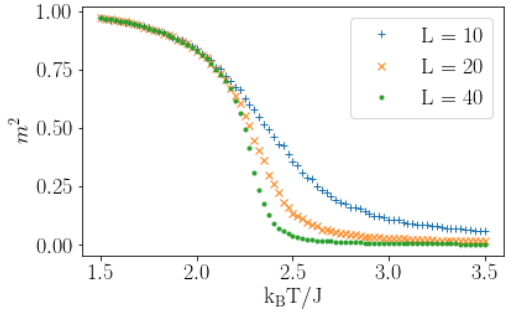

Figure 2. Averaged squared magnetisation near the critical temperature for different system sizes. Varying from $L = 10$ up to $L = 40$. Error bars are omitted as the standard deviation is small ($\sigma < 1\%$).

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 and thus figure 2.

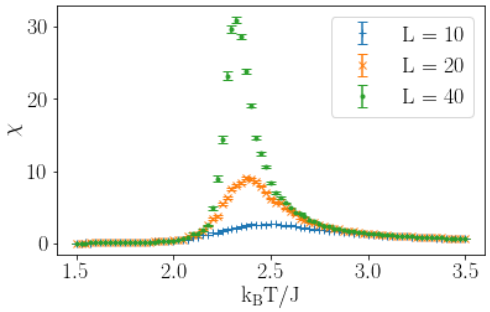

Figure 3. The magnetic susceptibility near the critical temperature for different system sizes.

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 $k_B T_c/J = 2.30(25)$. The uncertainty in T_c is fully determined by the temperature resolution which is 0.025.

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. 9 results 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.

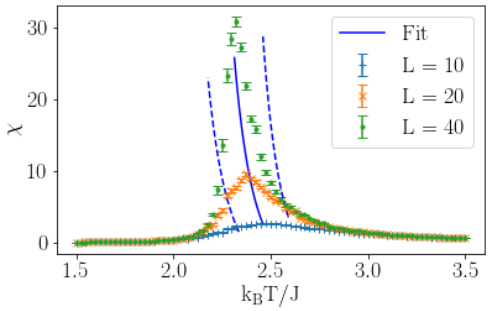

Figure 4. The fit is acquired from the full L-range ($10 - 40$, $\Delta L = 5$). Three system sizes are plotted to show the overall behaviour. The dotted blue lines represent the error in the fit.

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 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.

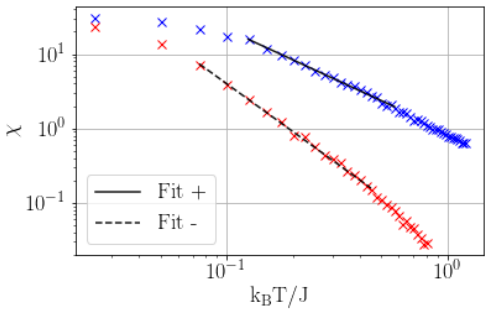

Figure 5. Logarithmic plot of χ including fit. For $(T-T_c) > 0$ χ is in blue with accompanying fit 'Fit +' and for $(T-T_c) < 0$ in red with 'Fit -'.

From figure 5, several observations can be made. The first one is the flattening of the curve for $|T - T_c|$ close to 0. The second observation is the presence of different slopes of the magnetic susceptibility 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.
In table 2 the found fit parameters are shown for both m and χ including the uncertainties.

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	$\beta = TBD(.)$	–
χ	$\gamma = ...(.)$	$\gamma = ...(.)$

The specific heat should have a relation as shown in table 1, but this was only possible for the $(T - T_c) < 0$ domain. The positive domain fitted better to a $(T - T_c)^a$ relation with $a \approx -0.5$. This is most likely caused by finite scale effect, but this must be investigated further.

Software performance

Fitting to normalised simulation time we learn that both algorithms scale quadratic in system size. The result is shown in figure 6. 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 they both have to scan the whole lattice to complete a MC step. 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. Making SW much more efficiënt. Both are linear in MC steps.

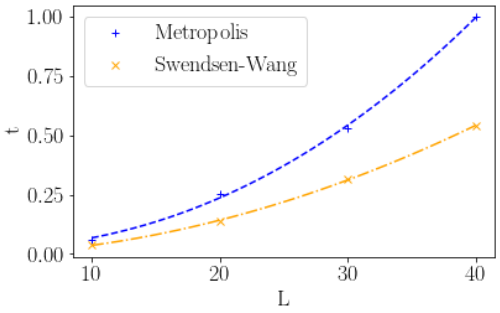

Figure 6. Normalised run time t with respect to system size $(L \times L)$ for both Metropolis and Swendsen Wang algorithm.

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 exponents for the physical quantities show some deviation from the infinite system limit, but this is most likely caused by the finite dimensions of the system. Further simulation for larger system sizes need to be done in order to confirm this suspicion. The dynamical critical exponent is determined in agreement with literature.

Reflection on cooperation

IN PROGRESS In general cooperation went well and quite a bit was learned along the way. It was noticed that it is important to first make a solid plan before the programming starts. In this plan there should be well defined tasks which can be made independently. For this we used a 'to-do' list application, but in the future we would like to start using the issue feature on Git. Besides that we were able to resolve the encountered problems together after discussing them. As for the workload, this was distributed as evenly as possible. During the intense week together the foundations was laid for a correct simulation after which the rest of the work to be done was divided per macroscopic quantity between each other. During the entire project results were discussed and

code was checked by each other. To give an overview of the specific distribution:

Together:
Tom:
Vincent:
Dit is de tekst van de vorige keer. Het is leuk als hiernaar wordt verwezen in de huidige cooperation tekst!!!

References

Ising, E. (1925, Feb 01). Beitrag zur theorie des ferromagnetismus. *Zeitschrift für Physik*, *31*(1), 253–258. Retrieved from https://doi.org/10.1007/BF02980577 doi: 10.1007/BF02980577

Onsager, L. (1944, Feb). Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Phys. Rev.*, *65*, 117–149. Retrieved from https://link.aps.org/doi/10.1103/PhysRev.65.117 doi: 10.1103/PhysRev.65.117

Swendsen, R. H., & Wang, J.-S. (1987, Jan). Nonuniversal critical dynamics in monte carlo simulations. *Phys. Rev. Lett.*, *58*, 86–88. Retrieved from https://link.aps.org/doi/10.1103/PhysRevLett.58.86 doi: 10.1103/PhysRevLett.58.86

Tang, S., & Landau, D. P. (1987, Jul). Monte carlo study of dynamic universality in two-dimensional potts models. *Phys. Rev. B*, *36*, 567–573. Retrieved from https://link.aps.org/doi/10.1103/PhysRevB.36.567 doi: 10.1103/PhysRevB.36.567

Thijssen, J. (2007). *Computational physics, 2nd edition*. Cambridge University Press.

Wimmer, M. T. (2018). *Course notes, project 2: Monte carlo simulations for the ising model.* Retrieved from https://gitlab.kwant-project.org/computational_physics_18/course_notes/blob/master/project%202/projects.md

Wolff, U. (1989). Comparison between cluster monte carlo algorithms in the ising model. *Physics Letters B*, *228*(3), 379 - 382. Retrieved from http://www.sciencedirect.com/science/article/pii/0370269389915633 doi: https://doi.org/10.1016/0370-2693(89)91563-3