# Computation Physics II 5640, Spring 2017

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## 1 Metropolis and Wolff algorithm for square lattice Ising model

We investigate the efficiency of two different algorithms for the time evolution of 2-D lattice models by studying the ferromagnetic Ising model on a square lattice. The Hamiltonian of the model is given by equation 1

$$\hat{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \tag{1}$$

where $\langle ij \rangle$ denotes neighboring pairs of spins $\sigma_i = \pm 1$, and $J$ is always positive for the ferromagnetic case.

We study the efficiency by comparing the temperature dependence of the energy density and the specific heat of the lattice, given by equation 2, respectively.

$$\frac{\left\langle \hat{H} \right\rangle}{N}, \qquad \frac{\beta^2}{N}\left(\left\langle \hat{H}^2 \right\rangle - \left\langle \hat{H} \right\rangle^2\right) \tag{2}$$

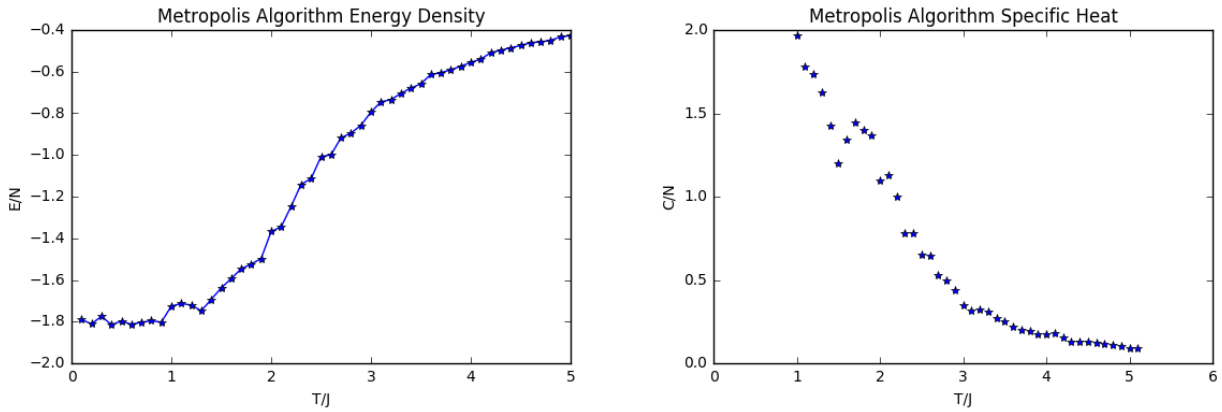
where $\langle ... \rangle$ denotes the monte-carlo average and $N$ is the number of spins.

### 1.1 Metropolis Algorithm

We implement the Metropolis algorithm by simulating 1000 $30 \times 30$ lattices, that are randomly seeded then allowed to simultaneously evolve in time for a particular temperature $T$, by the algorithm,

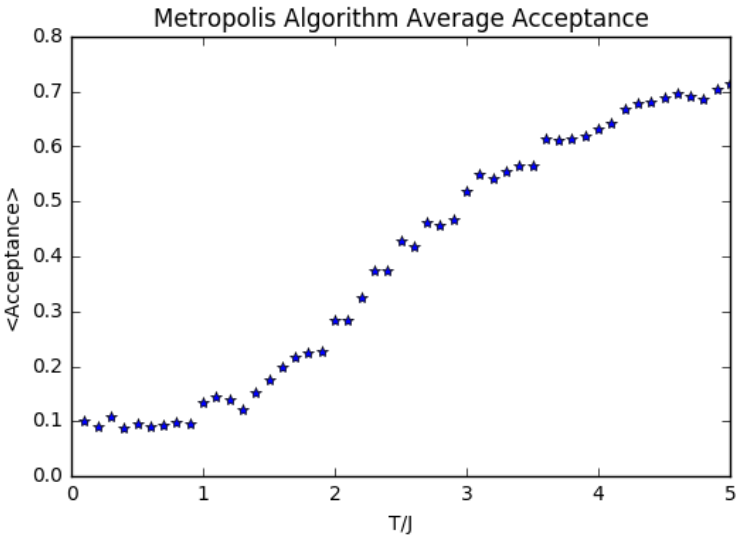
1. Choose a random site $i$,
2. Calculate the molecular field around the site, $H_{mol} = \sum_{\langle j \rangle} J\sigma_j$, where $\langle j \rangle$ is the set of neighboring pairs around $i$,
3. Throw a random number between zero and one, and if it is less than $exp(-\beta \Delta E)$, where $\beta$ is the inverse temperature, and $\Delta E = 2\sigma_i H_{mol}$, then flip $\sigma_i$.

We implement this algorithm for all 1000 lattices until a steady state is reached. It is here that we reveal that the efficiency is so bad for this algorithm, that on the time scales available, we were never actually able to reach the true steady state and get accurate results for the energy density, or the specific heat. Figures 1 (a), and 1 (b) show the results, but they do not have any relation to the real temperature distributions at low temperature. The reason for this is simple, at low temperatures, the value of $exp(-\beta \Delta E)$ is incredibly low, so almost no flips get accepted and the true steady state is not reached in a reasonable time. The acceptance distribution can be seen in figure 2 and the problem becomes obvious. The efficiency is better after the phase transition, where the distributions do resemble the accurate curves, but the plots are already ruined by then.




(a) (b)

Figure 1: Plots of energy density and specific heat for the Metropolis Algorithm. $N = 30^2$, $J = 1$




(a)

Figure 2:

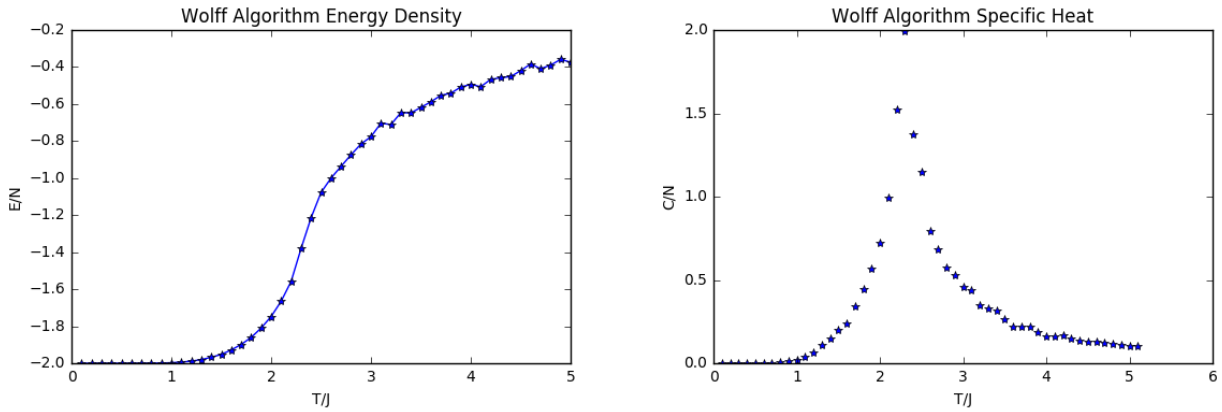
## 1.2 Wolff Cluster Algorithm

We implement the Wolff Cluster algorithm by simulating 1000 $30 \times 30$ lattices, that are randomly seeded then allowed to simultaneously evolve in time for a particular temperature $T$, by the algorithm,

1. Choose a random root site $i$, create a cluster array and an F array with $i$ included, and an empty F_new array,
2. For every site, j, in F, check the neighbors, k, of j and if $\sigma_j == \sigma_k$ and j is not already in the cluster then throw a random number between zero and one and if it is less than $1 - exp(-2\beta J)$ then add j to F_new and the cluster,
3. Replace F, i.e. all sites to check on next iteration, with F_new, and empty F_new,
4. Repeat items 2 and 3 until F is empty, i.e. there are no new sites with neighbors that could be added to the cluster,
5. Flip every spin in the cluster.

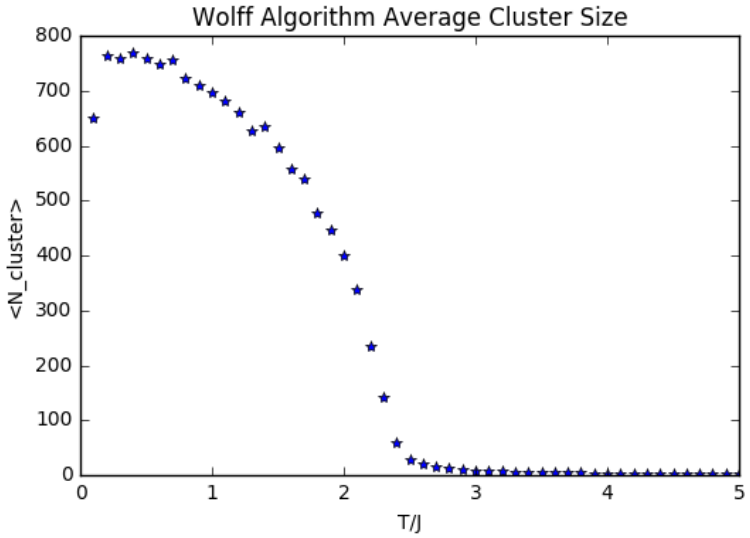
We implement this algorithm for all 1000 lattices until a steady state is reached. The results are presented in figure 3

We expected the plots from section 1.1 to closely match these, but that is obviously not the case. The Metropolis algorithm could not achieve the steady state at low temperatures even at 1000000 iterations, but the Wolff algorithm could reach it within 20 iterations at low temperature. The number of iterations needed increased with temperature, but never to the limits of the Metropolis algorithm. This behavior is understandable when figure 4 is inspected.




(a) (b)

Figure 3: Plots of energy density and specific heat for the Wolff cluster Algorithm, where we see the $-2J$ low temperature limit expect for the $J = 1$ case. We also see the specific heat have a discontinuity at the phase transition, as expected at the point where the energy density gradient spikes at a little over $T/J = 2$. $N = 30^2$




(a)

Figure 4:

The average cluster size is very high at low temperatures ($> 2/3$ of all spinors), and with every spin in the cluster being flipped, and the algorithm prioritizing spins being in the same direction, then you can expect it to be very efficient at low $T$. At the phase transition the cluster size shrinks considerably, but the steady state is not that far from the random state, so the efficiency is not an issue.