Cluster algorithms for the Ising model

Monte Carlo methods which overcome the problem of critical slowing down close to second order phase transitions

Contents

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- Phase transitions

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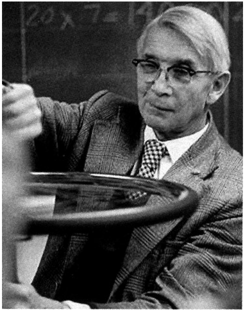

Figure : Ernst Ising (1900 - 1998)

Ising model - Definition

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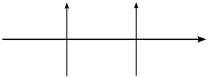

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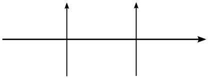

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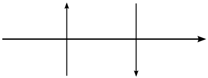

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$$p(\sigma, T) = \frac{e^{-\beta\mathscr{H}(\sigma)}}{\mathscr{Z}(T)}, \qquad \beta = \frac{1}{k_B T}$$

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$$\langle M \rangle_T = \sum_{\sigma} M(\sigma) p(\sigma, T)$$

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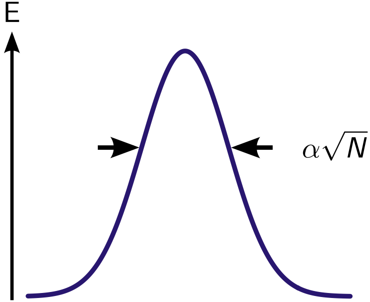

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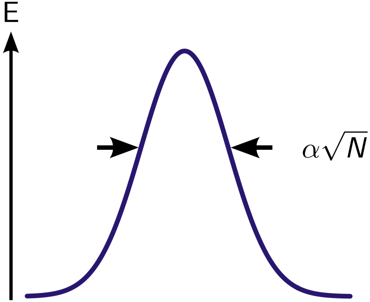

- Solution: Importance sampling using Metropolis algorithm

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Single spin flip metropolis - Algorithm

$$
\begin{aligned}
A(X \to Y) &= \min\left(1, \frac{p(Y)}{p(X)}\right) \\
&= \min\left(1, e^{-\beta[E(Y)-E(X)]}\right)
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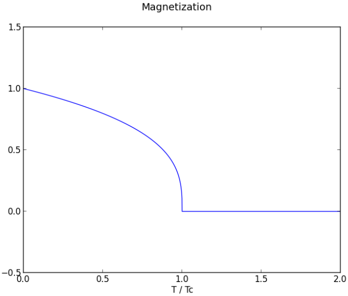
Expected



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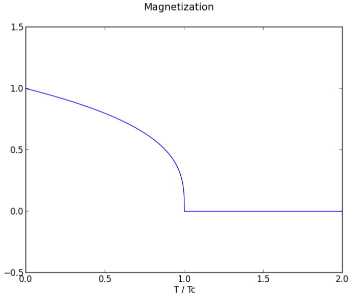
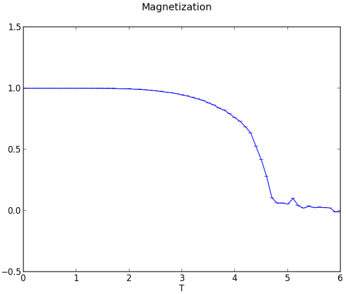


Obtained



Ising model - 2 spins

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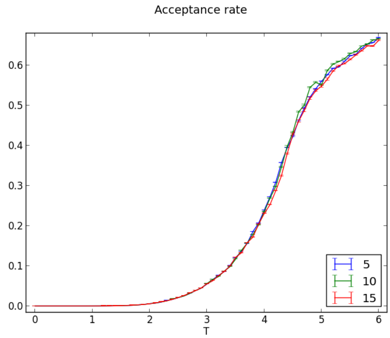

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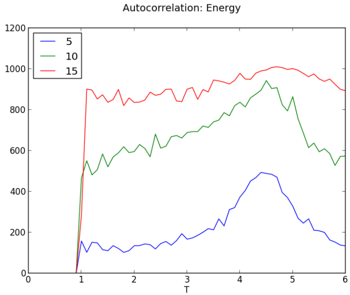

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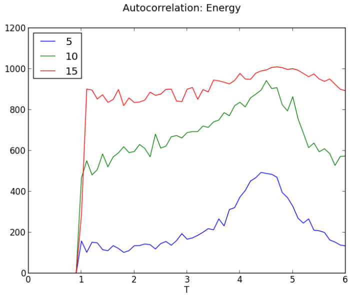

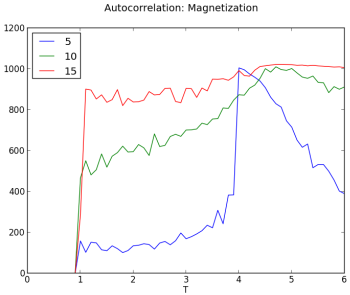

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$$\tau_X := \frac{\sum_{i=1}^{N}\sum_{t}\left(E\left[X_i X_{i+t}\right] - E\left[X\right]^2\right)}{\mathrm{Var}X}$$

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$$\tau_A = \lim_{l\to\infty}\left(\frac{2^l\mathrm{Var}A^{(l)}}{\mathrm{Var}A^{(0)}} - 1\right)$$

What really happens in the System

Cluster algorithms: Wolff algorithm

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Cluster algorithms: Wolff algorithm

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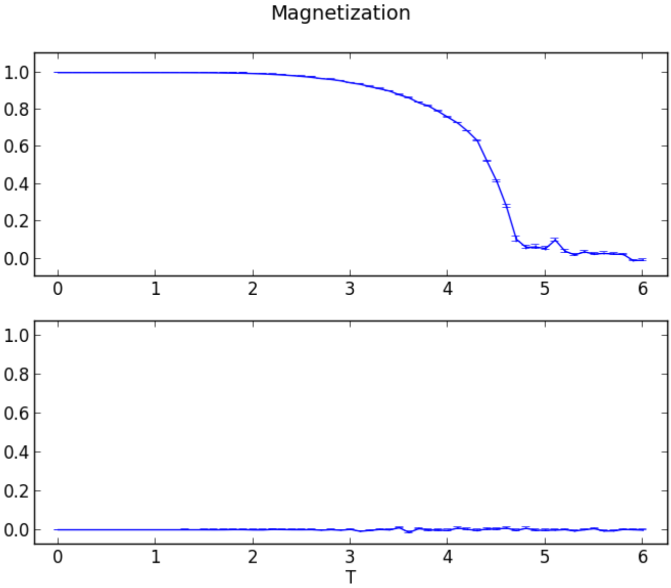
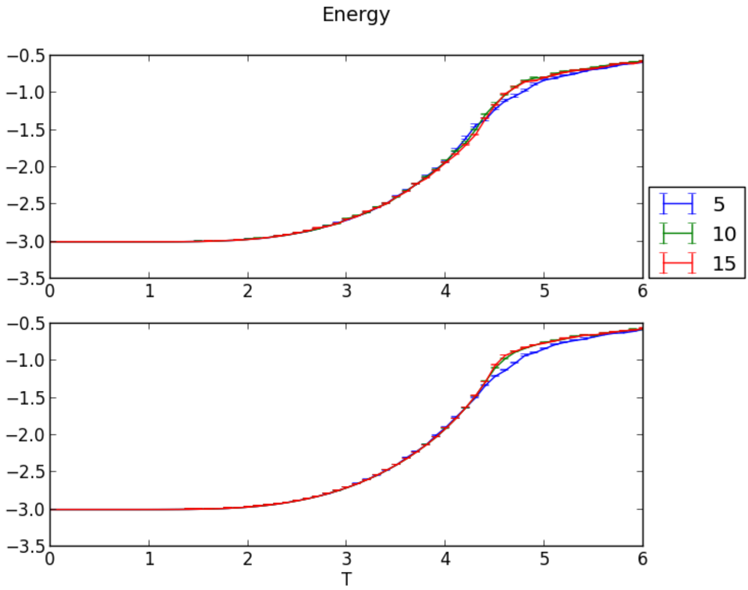
1. Choose one site (uniformly randomly)
2. Flip its spin and add it to the cluster
3. For all sites in the cluster:
   3.1 Visit every unknown neighbour, flip its spin and add it to the cluster with probability given above

Why cluster algorithms are better



Energy



Cluster size

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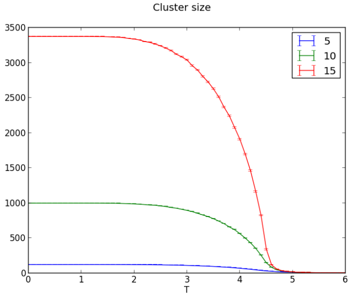

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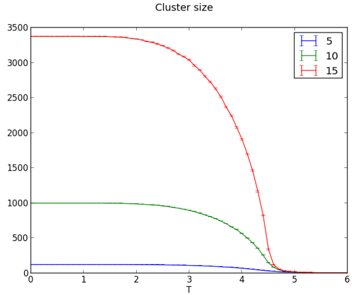
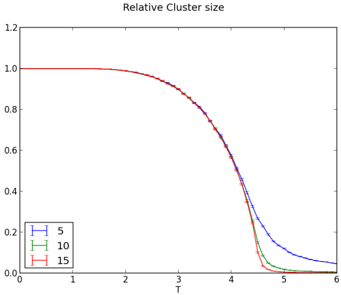
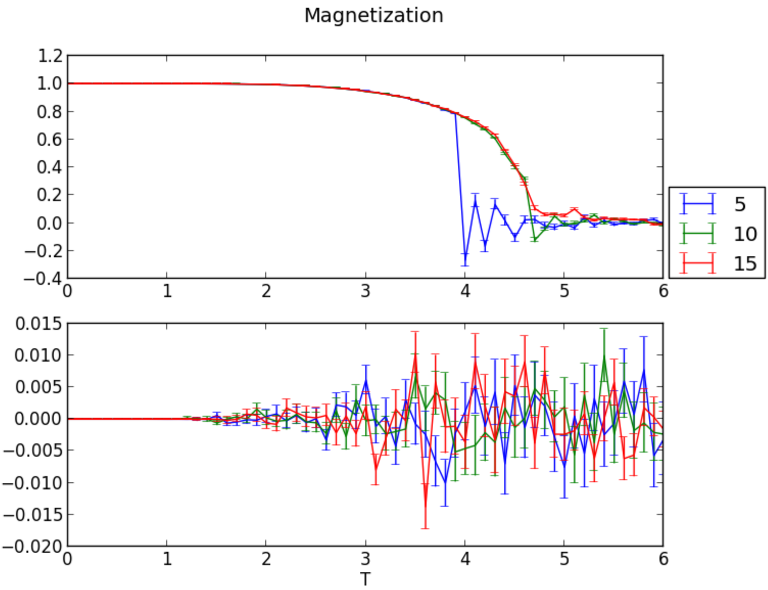
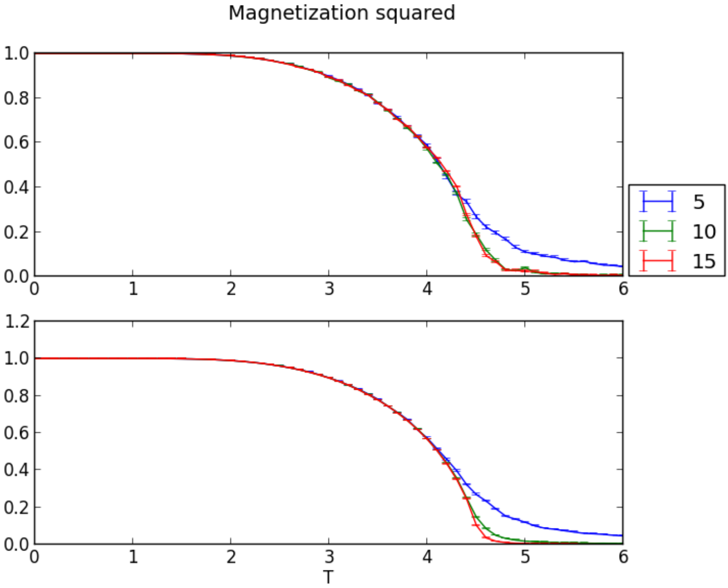




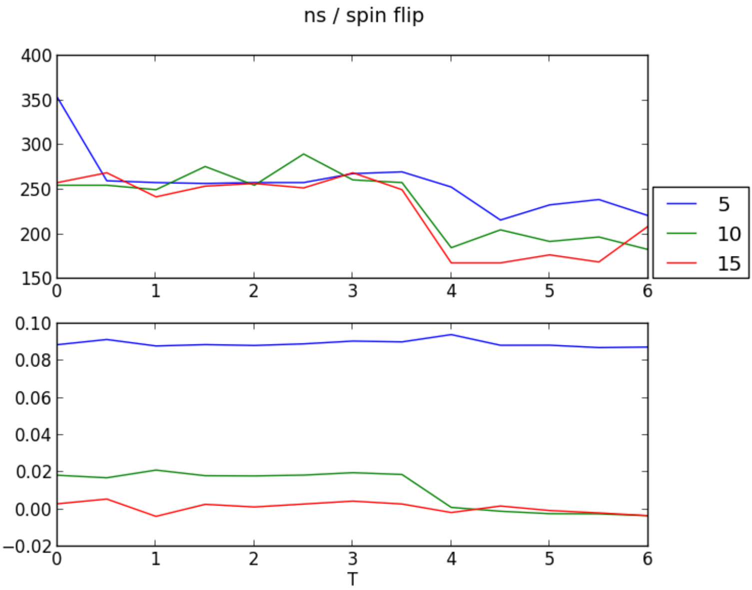
Magnetization



Magnetization squared



Computation time per spin flip



Swendsen-Wang

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Swendsen-Wang

Similar to Wolff, but:

- Partitions the whole lattice in clusters
- Randomly chooses a new (same) spin for every cluster
- Always touches every spin

Summary

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- Swendsen-Wang

References

- R.H. Swendsen and J-S. Wang, Phys. Rev. Lett. 58, 86 (1987)
- U. Wolff, Phys. Rev. Lett. 62, 361 (1989)

Questions

Binning analysis in detail

$$\mathrm{Var}X := E\left[X^2\right] - E\left[X\right]^2$$

$$\begin{aligned}
(\Delta X)^2 &= \frac{1}{N^2} \sum_{i,j=1}^{N} \left(E\left[X_i X_j\right] - E\left[X\right]^2 \right) \\
&= \frac{\mathrm{Var}X}{N} + \frac{1}{N^2} \sum_{i \neq j} \left(E\left[X_i X_j\right] - E\left[X\right]^2 \right) \\
&= \frac{\mathrm{Var}X}{N} + \frac{2}{N^2} \sum_{i=1}^{N} \sum_{t} \left(E\left[X_i X_{i+t}\right] - E\left[X\right]^2 \right) \\
&:= \frac{\mathrm{Var}X}{N} \left(1 + 2\tau_X\right)
\end{aligned}$$

Wolff or Swendsen-Wang?

Swendsen-Wang better for parallelization because it touches the whole lattice.