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Cluster Algorithms

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Introduction

- So far we have only encountered Monte-Carlo simulations on lattices with simple local objects, or off-lattice simulations where the particles could be moved locally.
- There exists the possibility of introducing changes in the configuration on a more global level.
- One of the problems, especially close to second-order phase transitions, is the critical slowing down. The system there behaves in a very correlated fashion. Local changes, as they are produced, for example with the Metropolis importance sampling, cannot propel the system fast enough through phase space.
- The result is a very slow relaxation into equilibrium and the continued large correlation between successive configurations.
- In the following example we want to examine a reformulation of the Ising model which will allow us to introduce larger changes to the configurations. This in turn leads to a reduction in the critical slowing down (1**?** ; 2).

Cluster Algorithm I

- The system for which we formulate the algorithm is the Ising model with the Hamiltonian

$$\mathcal{H}_{Ising} = -J \sum_{i,j} s_i s_j \tag{1}$$

  which we have met before several times.
- The main idea was put forward by Fortuin and Kastelyn (3). They proposed, and succeeded in showing, that the Ising model Hamiltonian could be mapped onto the percolation problem.
- The mapping gives a new partition function

$$Z = \sum_{n} B(\beta, n) 2^{c(n)} \tag{2}$$

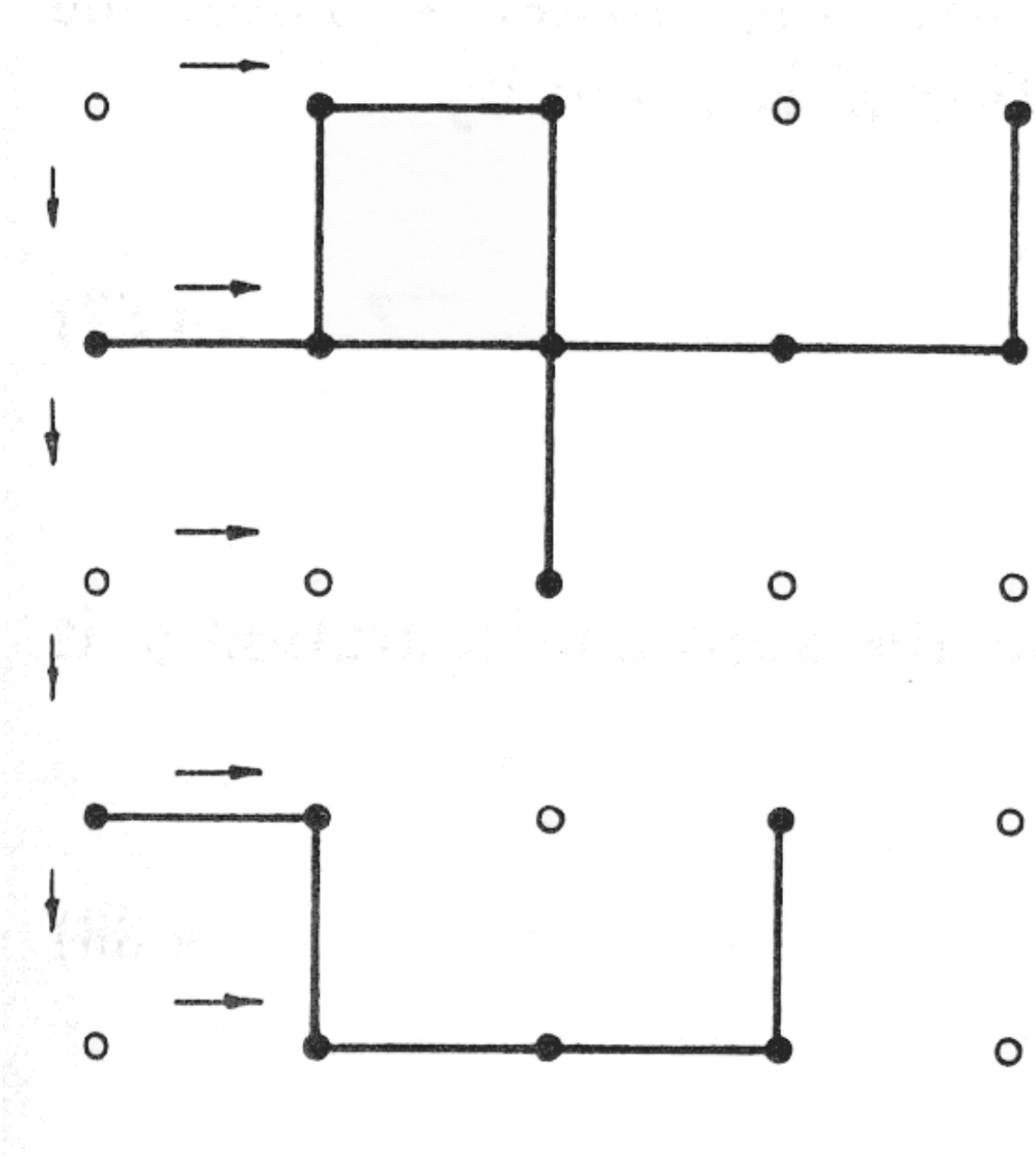
  i.e., a combinatorial factor and contributions from the two possible cluster orientations. Instead of single spins we now have to talk about patches, or clusters of spins. Each cluster is independent of the other clusters.

- To perform a Monte-Carlo simulation using this idea Swendsen and Wang (1) designed an algorithm to produce the clusters and to go from one configuration to another.

Cluster Algorithm II

- A configuration in the Swendsen-Wang method consists of an assignment of spin orientations to the lattice sites and an assignment of bonds between parallel spins.
- Consider such a configuration of a lattice with spin up and spin down.
- On top we have the bonds which are always broken between spins of opposite direction.
- Between spins of the same direction a bond can be present.
- A cluster is defined as follows: Two up spins belong to the same cluster if they are nearest neighbours and if there is a bond between them.

Cluster Algorithm III



Cluster Algorithm I

- Once all clusters of up spins and all clusters of down spins have been identified we can proceed to generate a new configuration.
- The first step consists in choosing a new orientation for each cluster.
- In the model without a magnetic field, the new orientation for each cluster is chosen at random, i.e., with a probability k the orientation is reversed.
- After this reorientation all bonds are deleted so that only the spin configuration remains.
- Now the process of a bond assignment and new cluster orientation is repeated.

- We shall now derive the probability with which we must assign a bond between parallel spins.
- Let us derive this for the Ising model with a magnetic field

$$\mathcal{H}_{Ising} = -J \sum_{\langle i,j \rangle} s_i s_j + \mu H \sum_i s_i \tag{3}$$

- Let $P(s) = Z^{-1} exp(-\beta \mathcal{H})$ be the probability for the occurrence of the configuration s. We shall define a new Hamiltonian

$$\hat{\mathcal{H}_{Ising}} = J \left[N_B - \sum_{\langle i,j \rangle} s_i s_j \right] + H \left[N_s + \sum_i s_i \right] \tag{4}$$

Cluster Algorithm II

- This Hamiltonian is zero for the ground state at zero temperature.
- Here N_B and N_S are the number of bonds on the lattice and the number of sites, respectively.
- Denote by $N_p(s)$ the set of all bonds that lie between two parallel spins and $c(\Gamma)$ the set of all closed bonds $[c(\Gamma)cN_p(s)]$.
- Define p to be the probability of the presence of a bond and q the absence of a bond.
- Then we have for the probability of getting a bond configuration Γ)

$$P(\Gamma) = \sum_s P(s)P(\Gamma \| s) \tag{5}$$

where the conditional probability that a bond configuration Γ is generated from a spin configuration s is

$$P(\Gamma \| s) = \delta_{\Gamma,s} p^{c(\Gamma)} q^{N_p(s)-c(\Gamma)} \tag{6}$$

- Assume we have a spin configuration.
- Choose the following spin orientations for the clusters λ
  - -1 with probability s = (I + exp[2pHN(A)])
  - +1 with probability t = 1 - s

where $N(\lambda)$ is the number of sites associated with the cluster λ.

Cluster Algorithm III

- Thus, the probability of generating a new spin configuration s' is given by

$$P(s') = \sum_{\Gamma} P(\Gamma) P(s' \| \Gamma) \tag{7}$$

  where $P(s' \| \Gamma)$ is the conditional probability that the spin configuration s' is generated from Γ, i.e.,

$$P(s' \| \Gamma) = \delta_{\Gamma, s'} s^{\gamma^-(\Gamma)} t^{\gamma^+(\Gamma)} \tag{8}$$

- with $\gamma^-(\Gamma)$ being the number of clusters of spin -1 and $\gamma^+(\Gamma)$ the number of clusters of spin $+1$.
- The total number of clusters is given by $\gamma(\Gamma) = \gamma^-(\Gamma) + \gamma^+(\Gamma)$
- We can now work out $P(\Gamma)$ and find that

$$q = exp\,(-2\beta J) \tag{9}$$

- Hence bonds are present on the lattice with $p = 1 - \exp(-2pJ)$ and clusters are reoriented with probability s.
- Finally the partition function for the normalized Hamiltonian is

$$\tilde{Z} = \sum_{\Gamma} p^{c(\Gamma)} q^{N_B - c(\Gamma)} \prod_{\lambda}^{\gamma(\Gamma)} [1 + exp(2\beta H N(\lambda))] \tag{10}$$

[1] R. Swendsen, Wang: Phys. Rev. Lett. 50,297 (1988)

[2] U. Wolff: Phys. Rev. Lett. 50,297 (1988)

[3] C.M. Fortuin, P.W. Kastelyn: Physica 57,536 (1972)