Cluster Simulations under a Constraint

Henk W.J. Blöte [†,‡], Youjin Deng [†], Jouke R. Heringa [†]

[†] Delft University, [‡] Leiden University

Outline:

1. Critical Slowing Down
2. Cluster Monte Carlo
3. Proof of detailed balance
4. The role of symmetry
5. The geometric cluster method
6. Fisher renormalization
7. Conclusion

1) Critical Slowing Down

Usually, simulations at criticality are *slow*.
Dependence on finite size L:

$$\tau_L \propto L^z$$

Computer time $\propto L^{d+z}$ per independent configuration in d dimensions. Typically, $z \approx 2$ for local updates:

$z = 2.1665(2)$ for 2-d Ising model (Metropolis)

However, see also

$z = 3.75$ for 2-d Ising model (Kawasaki dynamics)

and

$z = 0$ for the percolation problem.

In general, critical slowing down restricts simulation to small L.

Local Ising update according to Metropolis:

i) select particle in state s_i
ii) propose new state $s_i' = -s_i$
iii) calculate energy change ΔE
iv) if $\Delta E \leq 0$, accept new state s_i';
if $\Delta E > 0$, accept new state with probability $\mathrm{e}^{-\Delta E/k_\mathrm{B}T}$.

spin is flippable if $\Delta E \leq 0$, and
if $\Delta E > 0$ it is flippable with probability $\mathrm{e}^{-\Delta E/k_\mathrm{B}T}$.

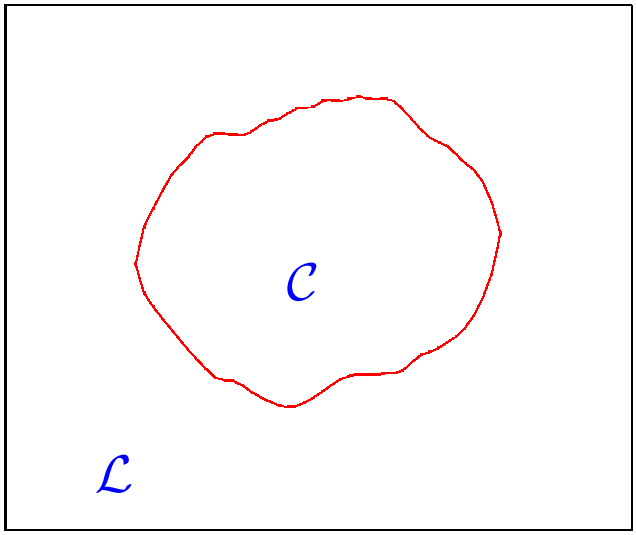
2) Cluster Monte Carlo

Ferro Potts model: Swendsen-Wang algorithm.
Clusters: groups of spins connected by rigid bonds.
Bonds: not rigid if they connect unequal spins.
Equal spins: rigid with probability $1 - \mathrm{e}^{-K}$
with $\Delta E/k_\mathrm{B}T = \pm K$. Similarity with local updates:

bond is flippable if $\Delta E \leq 0$;
if $\Delta E > 0$, flippable with probability $\mathrm{e}^{-\Delta E/k_\mathrm{B}T}$.

3) Detailed Balance

Consider single-cluster version (Wolff):
Cluster $\mathcal{C}$: all sites connected by rigid bonds.
Flip cluster $\mathcal{C}$: configuration $\Gamma \to \Gamma'$



Probability of this cluster flip:

$$T(\Gamma', \Gamma) = P_{\text{internal}}(\Gamma, \mathcal{C})\; P_{\text{boundary}}(\Gamma, \mathcal{C})$$

P_{internal}: probability that all sites in $\mathcal{C}$ are connected;
P_{boundary}: that no site outside $\mathcal{C}$ is connected.

Thus $\boxed{P_{\text{boundary}} = \exp[-\sum{}^{+} \Delta E / k_{\text{B}} T]}$
where $\sum^{+} \Delta E$ collects the energy changes of bonds whose energy *increases* when $\Gamma \to \Gamma'$.

Next: probability of inverse flip $\Gamma' \to \Gamma$:

$$T(\Gamma, \Gamma') = P_{\text{internal}}(\Gamma', \mathcal{C}) P_{\text{boundary}}(\Gamma', \mathcal{C})$$

or

$$T(\Gamma, \Gamma') = P_{\text{internal}}(\Gamma, \mathcal{C}) \exp[-\sum{}^{+} \Delta E'/k_{\text{B}}T]$$

where $\sum^{+} \Delta E'$ collects the energy changes of bonds whose energy *increases* when $\Gamma' \to \Gamma$.
Thus

$$T(\Gamma, \Gamma') = P_{\text{internal}}(\Gamma, \mathcal{C}) \exp[+\sum{}^{-} \Delta E/k_{\text{B}}T]$$

where $\sum^{-} \Delta E$ collects the energy changes of bonds whose energy *decreases* when $\Gamma \to \Gamma'$.
Taking the ratio leads to

$$\begin{aligned} \frac{T(\Gamma', \Gamma)}{T(\Gamma, \Gamma')} &= \exp[-(\sum{}^{+} \Delta E + \sum{}^{-} \Delta E)/k_{\text{B}}T] \\ &= \exp[-\{E(\Gamma') - E(\Gamma)\}/k_{\text{B}}T] \end{aligned}$$

This proves the condition of detailed balance.

4) The role of symmetry

Essential requirements for the proof of detailed balance are:

- The 'flipping' of a cluster corresponds with a global symmetry, e.g. permutation symmetry in the case of the Potts model. $\mathcal{H}$ must be invariant under this symmetry.

- the symmetry operation must be its own inverse.

Another (implicit) condition is that there are only pair interactions. Any model with a symmetry satisfying these conditions can be simulated by a cluster Monte Carlo method.

5) The geometric cluster Monte Carlo method

Consider a self-inverse geometric symmetry operation interchanging lattice sites i and i', j and j', etc. These operations can be:

- translations over half the system size (in case of pbc),
- rotations over π,
- mirror inversions,
- and combinations of these.

In many cases the Hamiltonian of a model satisfies such global symmetries, and a cluster Monte Carlo algorithm can be formulated. See:

continuous space:	Dress & Krauth, J. Phys. A **28** L597 (1995)
lattice models:	Heringa & Blöte, Physica A **232** 369 (1996)
2 lattice models:	Redner et al., Phys. Rev. E **58** 2749 (1998)

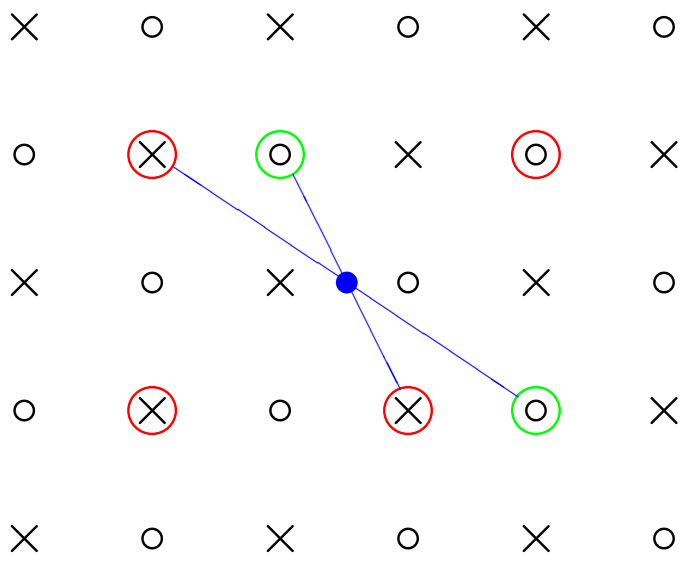
Cluster formation rule:

bond pair is flippable if $\Delta E \leq 0$;
if $\Delta E > 0$, flippable with probability $e^{-\Delta E/k_B T}$.

Examples:

- Ising and Potts models at nonzero magnetization
- lattice gases with nearest-neighbor exclusion
- critical and tricritical Blume-Capel model (spin-1 Ising model)
- Potts models with vacancies
- Baxter's hard-square and hard-hexagon lattice gases

Example of geometric cluster formation:



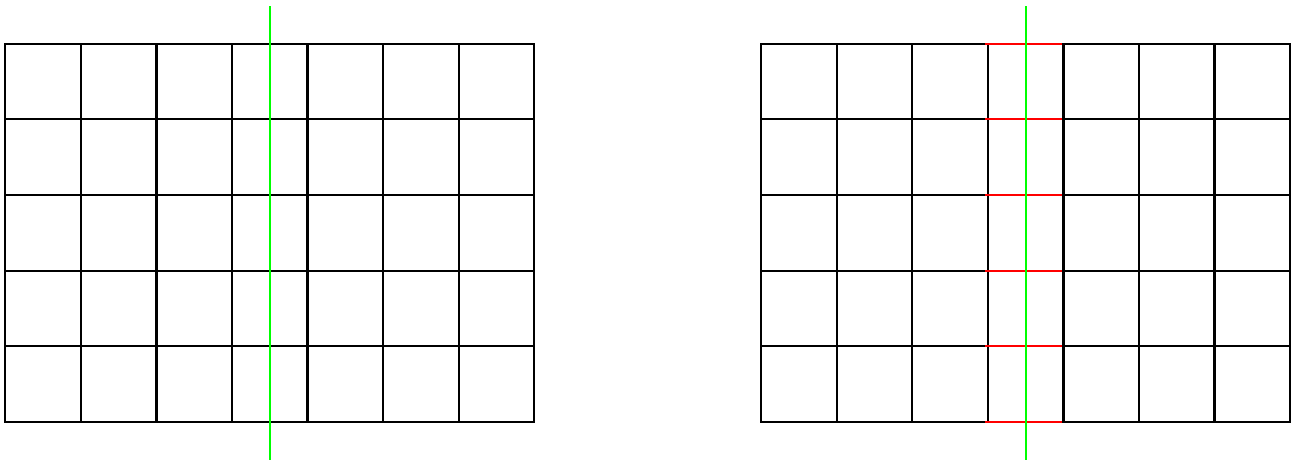
Hard-square LG

Critical slowing down if only clusters

- of size of order 1
- of size of order L

Optimal efficiency if cluster formation occurs *on percolation threshold*

Proof for 2-D ferro Ising model:



L R

One system (R) has AF seam (red lines).
Fold lattices: $\rightarrow$ $++$, $+-$, $-+$, and $--$ pairs.
Critical susceptibility of L^d system:

$$\chi(L) = N^{-1}\langle (N_{++} - N_{--})^2 \rangle \propto L^{2y_h - d}$$

for both systems L and R. Add indices:

$$\begin{aligned} \chi_{\mathsf{R}}(L) &= N^{-1}\langle (N_{++} - N_{--})^2 \rangle_{\mathsf{R}} \\ &= N^{-1}\langle (N_{+-} - N_{-+})^2 \rangle_{\mathsf{L}} \end{aligned}$$

Form S-W style geometric clusters on L
using mirror inversion (green line)

There are 2 sorts of clusters:

- 2-spin clusters: $++$ or $--$ pairs;
- others: $+$ spins in one sheet, $-$ spins in other.

Let there be n_c 'other' clusters. Since $+-$ and $-+$ are equally probable, one has

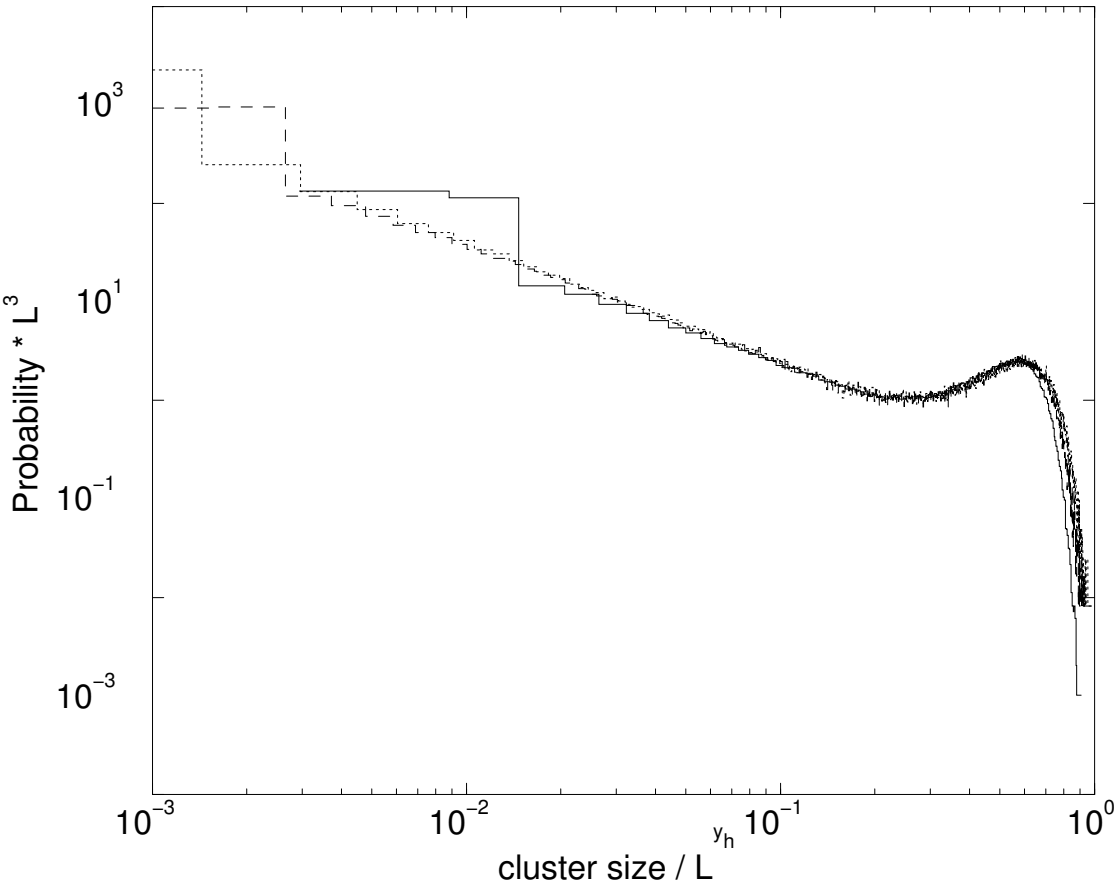
$$N^{-1}\langle (N_{+-} - N_{-+})^2 \rangle = N^{-1}\, 2^{-n_c}$$

$$\langle \sum_{s_1=\pm 1} \cdots \sum_{s_{n_c}=\pm 1} (\sum_k n_k s_k)^2 \rangle = N^{-1} \langle \sum_k n_k^2 \rangle$$

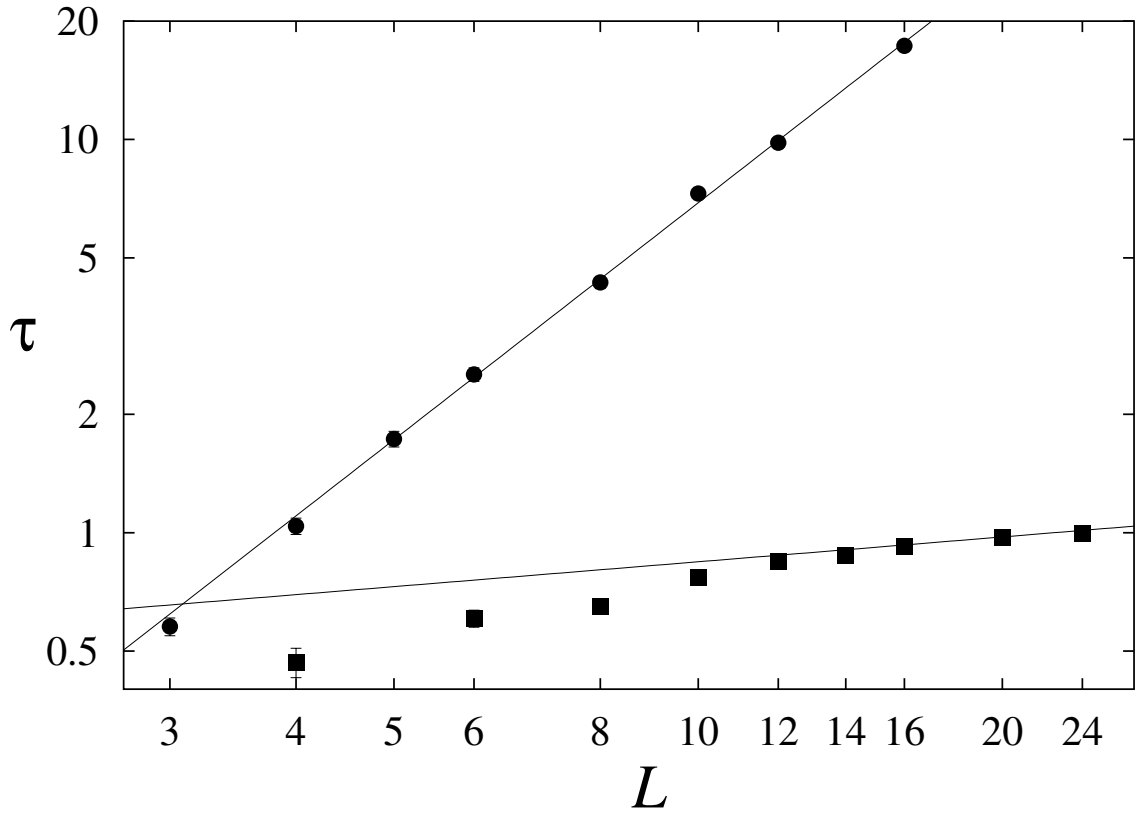
Since probability to select cluster k is n_k/N, this is the *average geometric cluster size* for the single-cluster method.
Recall:

$$\chi \propto L^{2y_h - d}$$

$\rightarrow$ percolation threshold.



Cluster size distribution for critical simple-cubic lattice gas with nn exclusion. System sizes are L^3 with $L =$8, 16 and 32.



Autocorrelation times τ of energy of tricritical 3D Blume-Capel model (Ising with vacancies)
circles: single-spin updates
squares: geometric clusters

Result $z \approx 0.21$ seems to violate Li-Sokal limit (Phys. Rev. Lett. **63**, 827 (1989)) which says
$z \geq \alpha/\nu = 1 \qquad (\alpha = \nu = 1/2)$
for tricritical 3D Ising model.
Way out: calculate α under *constraint*: $\alpha = -1$.

6) Fisher Renormalization

Constraint: scaling properties modified. Example: Blume-Capel model (s =1 Ising):

$$\mathcal{H} = -K \sum_{<ij>} s_i s_j + D \sum_k s_k^2$$

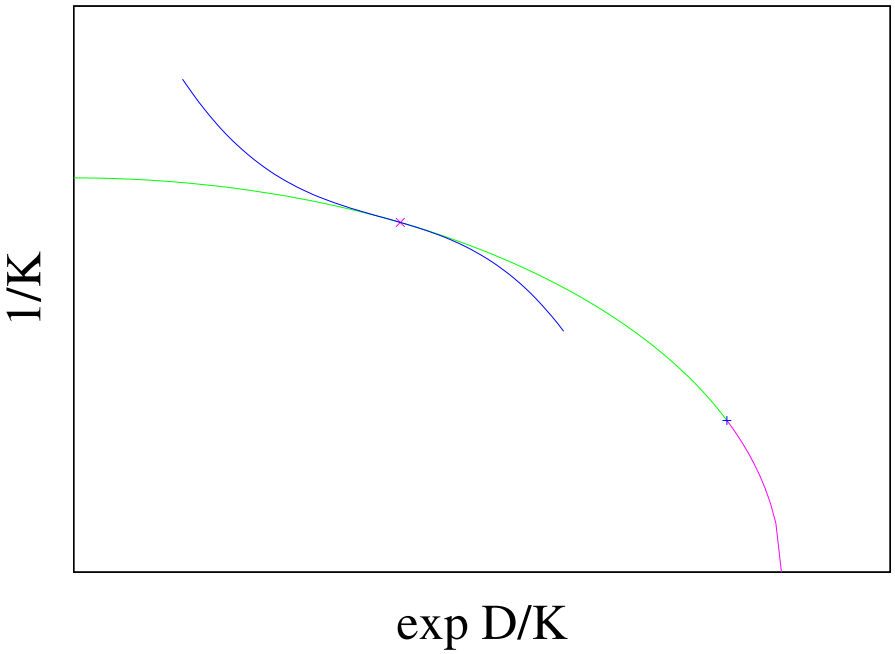
with $s_l = \pm 1$ or 0. The canonical partition sum is

$$Z = \sum_{\{s_i\}} \exp(-\mathcal{H})$$

under the restriction that there are N_v vacancies:

$$Z(N_v) = \sum_{\{s_i\}} \delta_{\sum_k s_k^2, N - N_v} \exp(-\mathcal{H})$$

we explore the *constant vacancy density* ensemble.



System describes path $D(K)$ determined by

$$\langle \sum_k s_k^2 \rangle = -\frac{\partial \log Z(K,D)}{\partial D} = N - N_v$$

Thermodynamic limit: M.E. Fisher, Phys. Rev. **176**, 257 (1968).

Finite-size-scaling: mostly unexplored.

7) Conclusion

- Cluster simulation of new models
- Investigation of constrained systems
- Exploration ‘new’ physics
- More applications are possible