Applications of Geometric Cluster Algorithms

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Outline:

1. Cluster Monte Carlo
2. Proof of detailed balance
3. The geometric cluster method
4. Fisher renormalization
5. Conclusion

Contributions from:

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1) Cluster Monte Carlo

Local updates at criticality are *slow*.
Autocorrelation time τ_L vs. system 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 $\mathrm{e}^{-\Delta E/k_{\mathrm{B}}T}$.

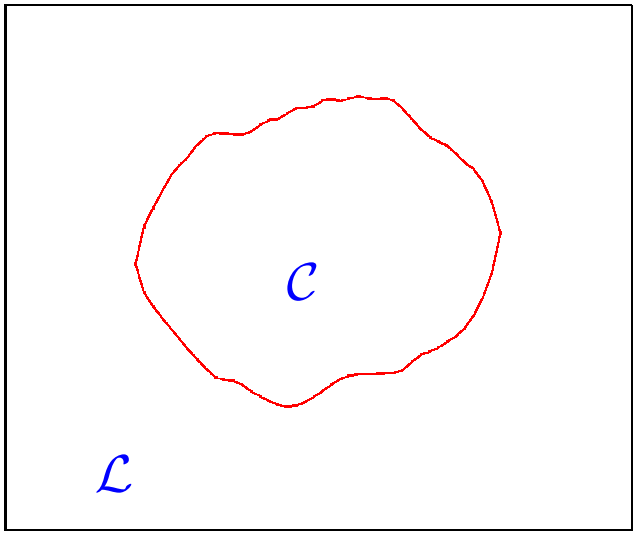
Cluster Monte Carlo:

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 $\mathrm{e}^{-\Delta E/k_{\mathrm{B}}T}$.

2) 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 is the condition of detailed balance.

The role of symmetry

Conditions for the proof of detailed balance:

- Cluster 'flips' correspond 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 self-inverse.

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

3) 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.

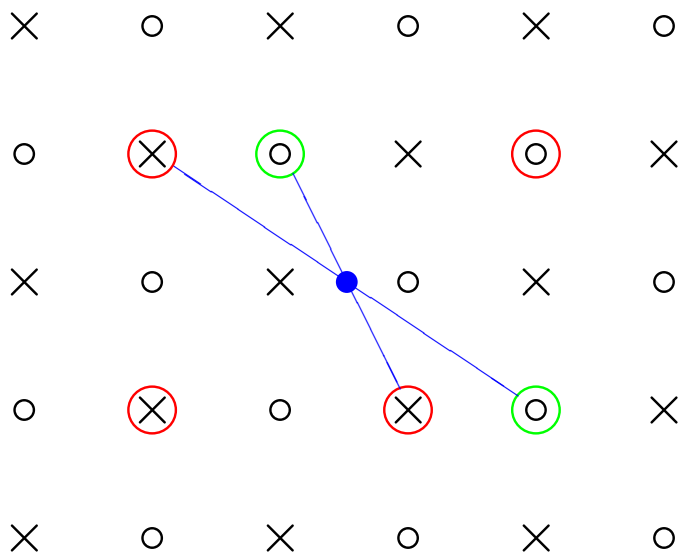
In many cases the Hamiltonian of a model satisfies such global symmetries, and a cluster Monte Carlo algorithm can be formulated. See:

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 cluster formation:



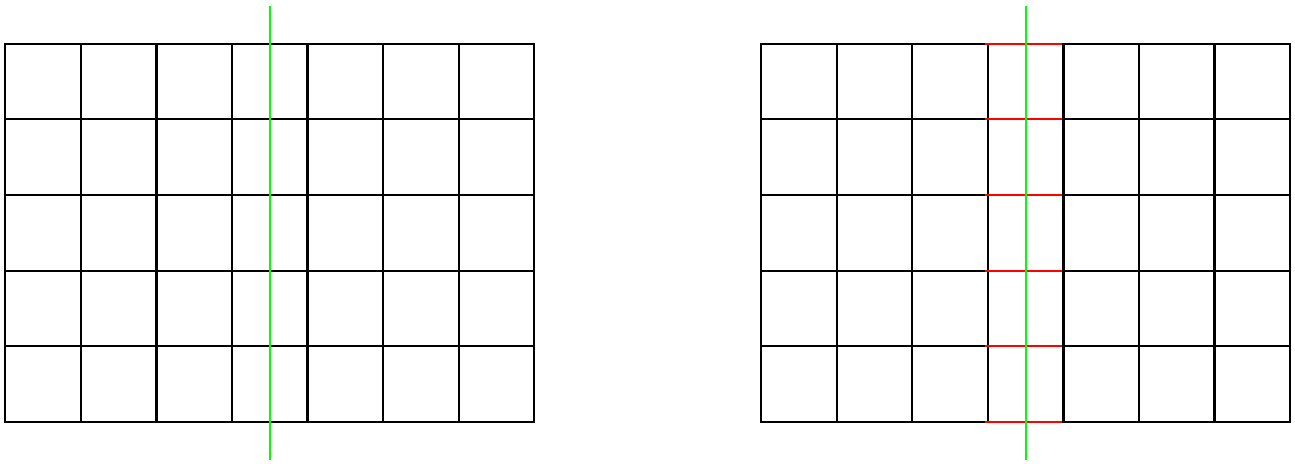
Formation of geometric cluster in hard-square LG

Critical slowing down? Yes, 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

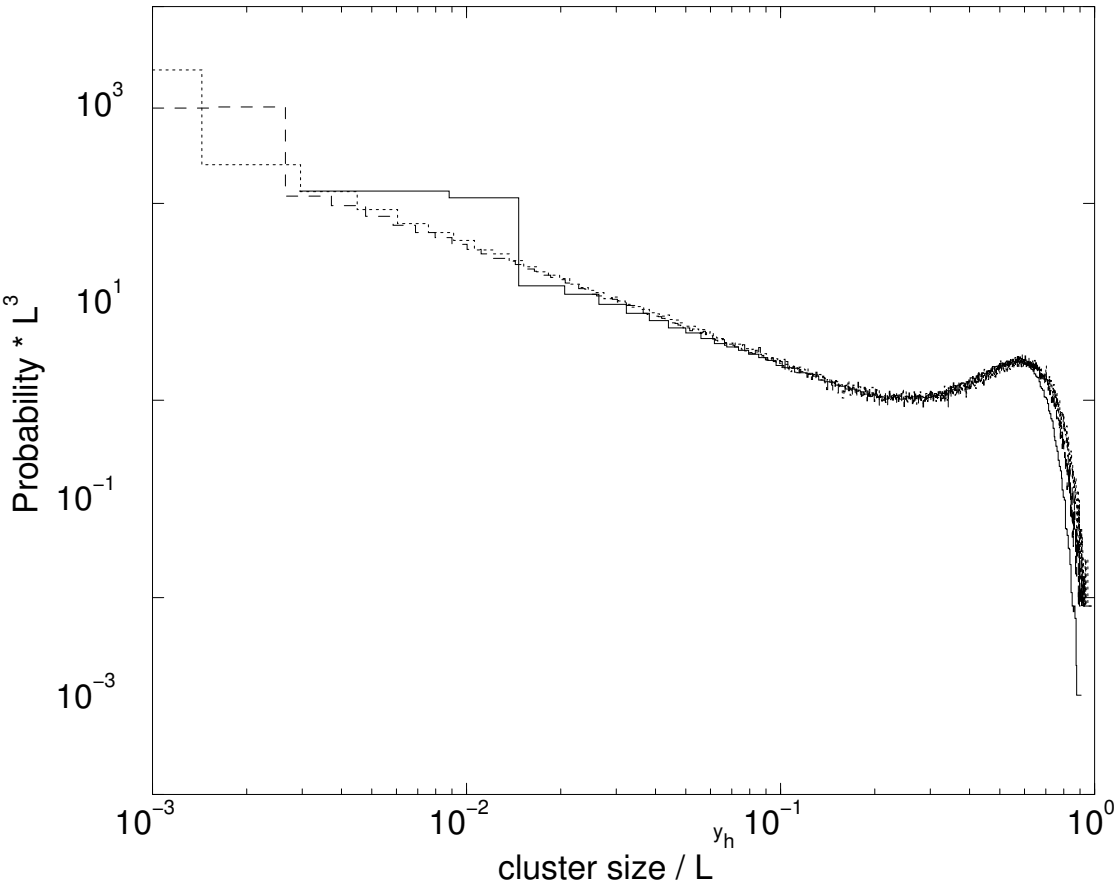
$$N^{-1}\langle (N_{+-} - N_{-+})^2 \rangle = N^{-1}\, 2^{-n_c}$$

$$\langle \sum_{p_1=\pm 1} \cdots \sum_{p_{n_c}=\pm 1} (\sum_k n_k p_k)^2 \rangle = N^{-1} \langle \sum_k n_k^2 \rangle$$

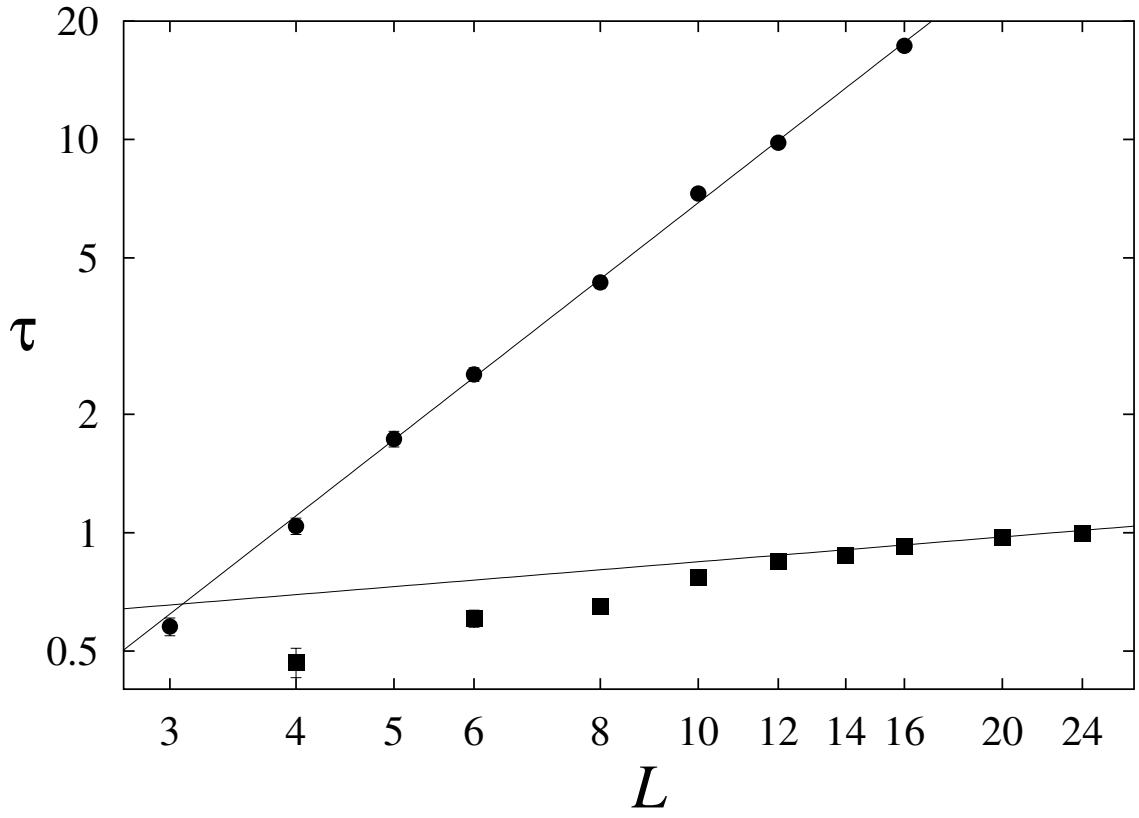
Since probability to select cluster k is n_k/N, this is the *average geometric cluster size* for the single-cluster method.
Recall:

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

$\rightarrow$ 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*: $\alpha = -1$.

4) 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. Grand canonical partition sum:

$$Z_{\mathrm{g}} = \sum_{\{s_i\}} \exp(-\mathcal{H})$$

Canonical partition sum for N_v vacancies:

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

explores the *constant vacancy density* ensemble.

Theory for thermodynamic limit:
M.E. Fisher, Phys. Rev. **176**, 257 (1968).
If one knows

$$F_{\mathsf{g}}(K,D) = -kT \ln Z_{\mathsf{g}}(K,D)$$

one can calculate

$$F_{\mathsf{c}}(K,\rho) = -kT \ln Z_{\mathsf{c}}(K,\rho)$$

because system describes path $D(K)$ determined by

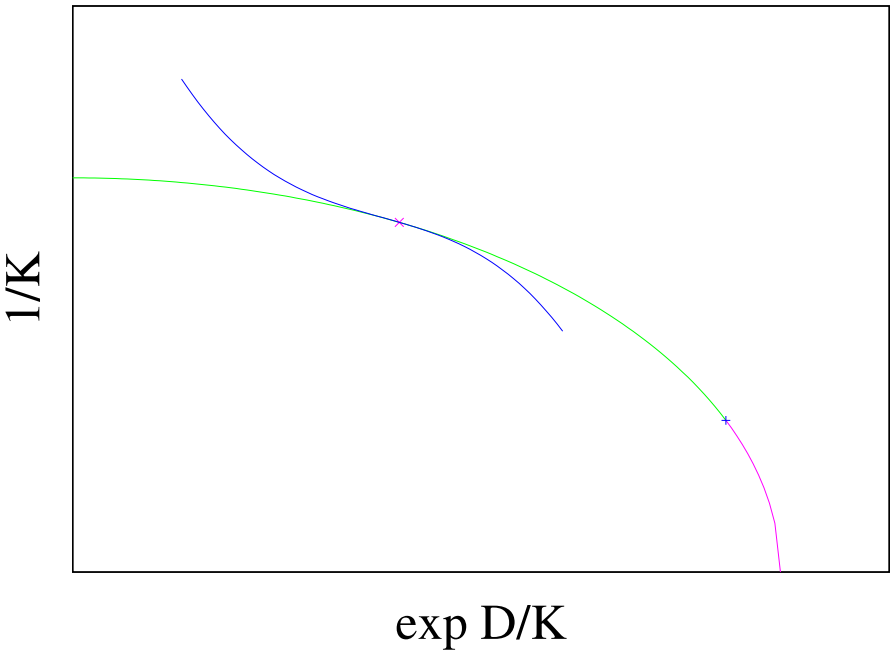
$$\langle \sum_k s_k^2 \rangle = -\frac{\partial \log Z(K,D)}{\partial D} = N - N_v$$

so that

$$\rho_{\mathsf{g}} = 1 + \frac{\partial \log Z(K,D)}{\partial D}$$

$$\rho(K, D) \to D(K, \rho)$$

Path of constrained system in (K, D) plane:



Substitute in F_{g}:

$$F_{\mathsf{g}}(K, D) = F_{\mathsf{g}}(K, D(K, \rho))$$

Thermodynamic limit: OK

Finite-size-scaling: mostly unexplored.

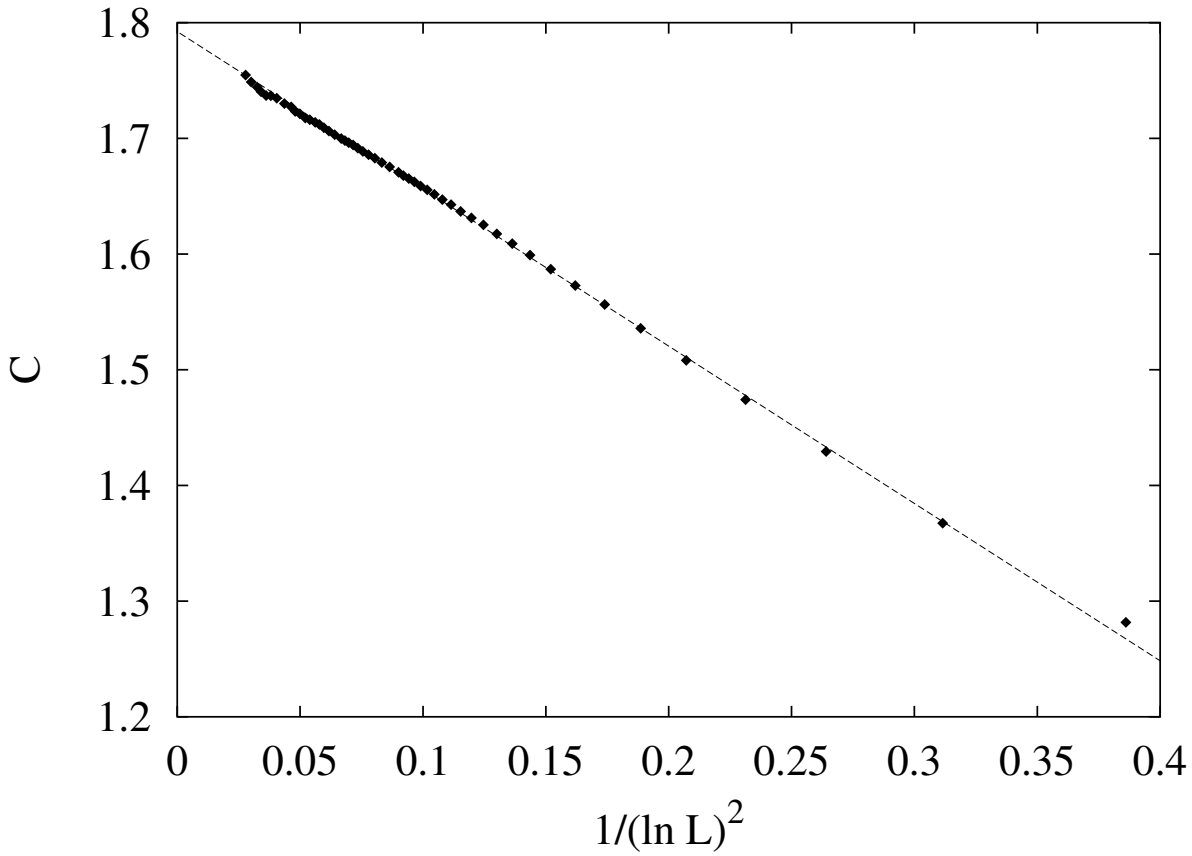
Constrained specific heat (Fisher renormalized):

$$C(L) = C_\infty + aL^{d-2y_t} \quad \text{if} \quad d - 2y_t < 0$$

For Ising case $d - 2y_t = 0$:

$$C(L) = C_\infty + a/\ln L + \cdots$$

However...



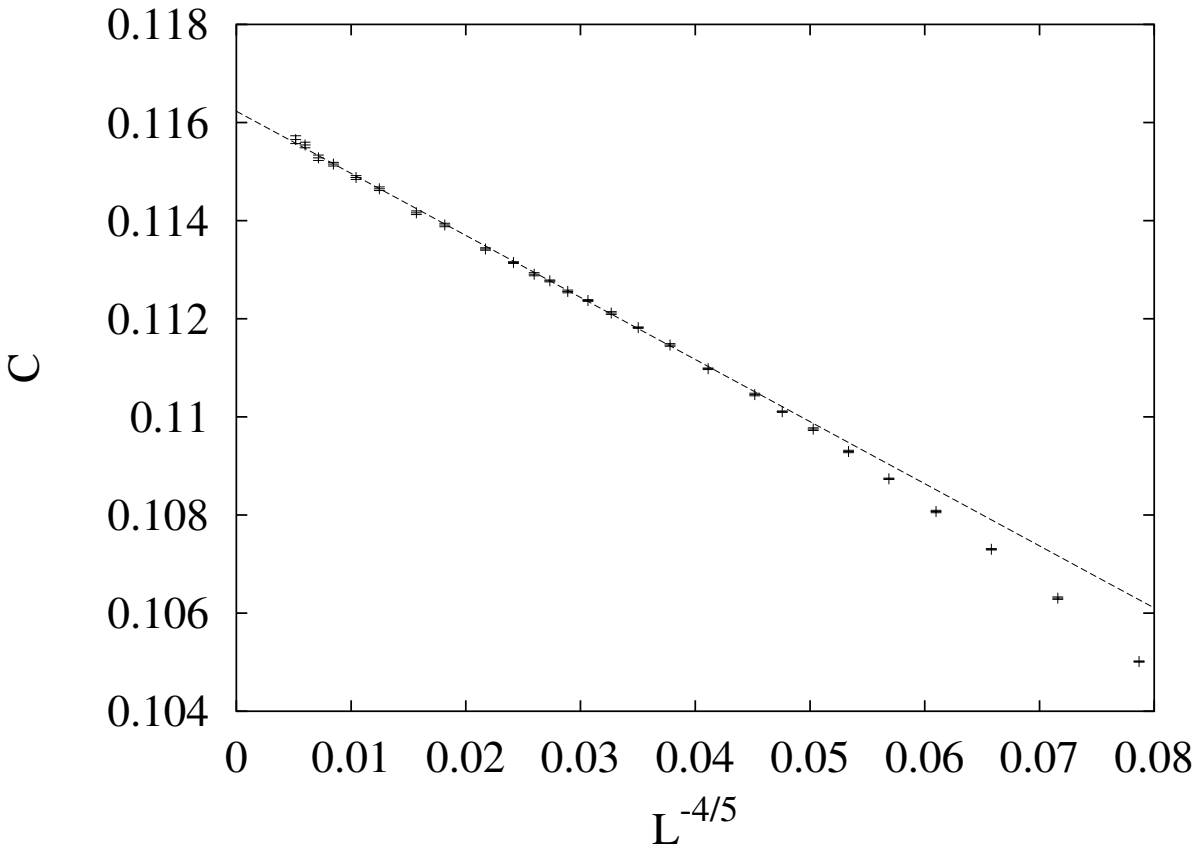
Constrained specific heat of critical Blume-Capel model vs. L

Hard-hexagon model: $y_t = 6/5$.

Fixed density: Fisher renormalization expected

$$C(L) = C_\infty + aL^{d-2y_t} = C_\infty + aL^{-2/5}$$

However...



Constrained specific heat of critical hard-hexagon model vs. L

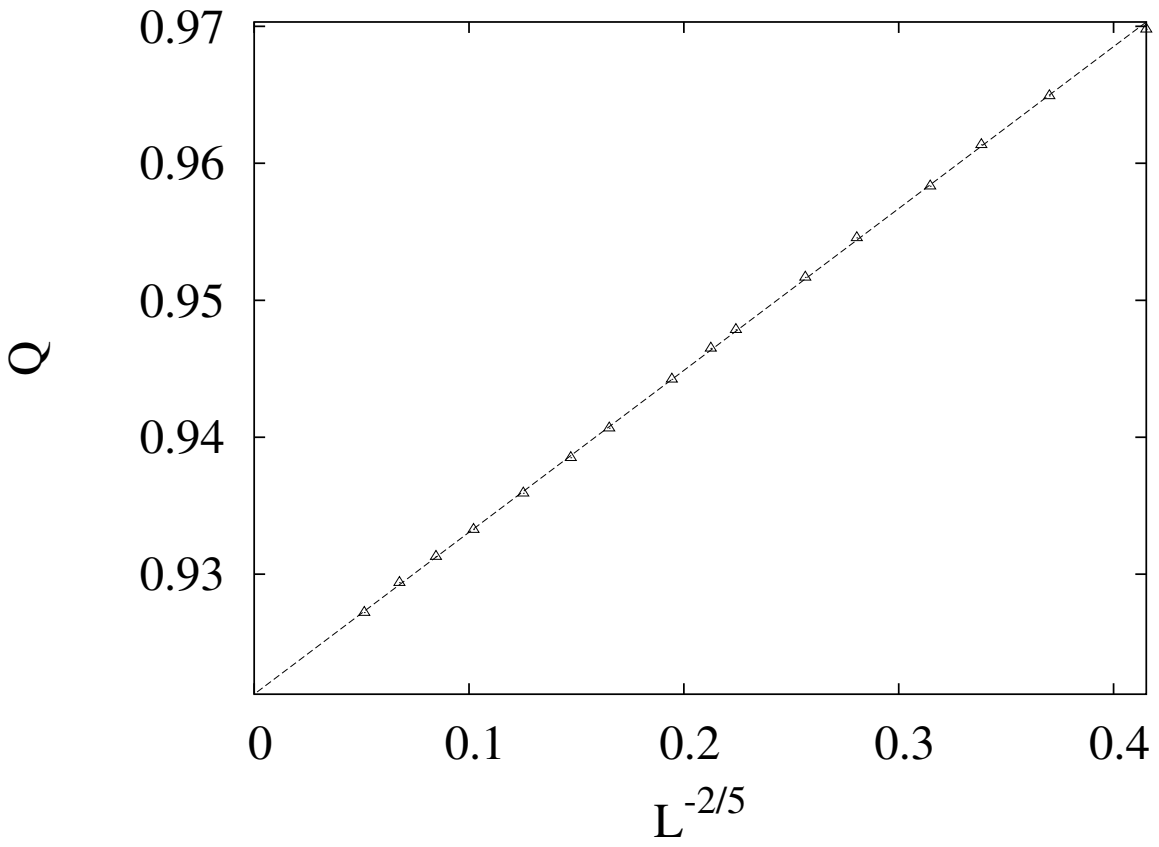
Amplitude ratio Q of dilute $q = 3$ Potts model with constrained vacancy density

$$Q \equiv \langle m^2 \rangle^2 / \langle m^4 \rangle$$

behaves, according to scaling, as

$$Q = Q_\infty + a L^{y_i}, \quad y_i = -4/5$$

However...



Critical amplitude ratio Q vs. L.

Explanation behavior Q;
Assume renormalization in grand ensemble

$$f(t,h,u,L) = -kT \ln Z_{\mathrm{g}}$$

$$= f_a + L^{-d} f(L^{y_t} t, L^{y_h} h, L^{y_i} u, 1)$$

exponents y_t etc. known in principle
Scaling behavior of observables follows:

$$Q_{\mathrm{g}} = Q_{\infty,\mathrm{g}} + a L^{y_i}\,, \quad y_i = -4/5$$

Q_{c} behaves near criticality as:

$$Q_{\mathrm{c}} = Q'_{\infty,\mathrm{c}} + a' L^{y_1} + \sum_k a_k (\Delta\rho)^k L^{k y_\rho}$$

where y_1 unknown;
$\Delta\rho =$ deviation w.r.t. critical density
$y_\rho = d - y_t$ if $2y_t - d \geq 0$
$y_\rho = y_t$ if $2y_t - d < 0$.

Grand canonical expectation value:

$$Q_{\mathsf{g}}(\mu,T) = \frac{\sum_{N_p}\sum_{\{\sigma\}}\delta_{N_p,\sum_k\sigma_k}Q(\{\sigma\})\exp[-\mathcal{H}]}{Z_{\mathsf{c}}} \times$$
$$\frac{Z_{\mathsf{c}}}{Z_{\mathsf{g}}} = \int \mathrm{d}\rho Q_{\mathsf{c}}(\rho,T)P(\mu,\rho)$$

insert expression for Q_{c} with
$\langle(\Delta\rho)\rangle = 0$ at criticality and
$\langle(\Delta\rho)^2\rangle = r_0 L^{-d} + r_1 L^{2y_t-2d}$
Leading order of $\Delta\rho$:

$$Q_{\mathsf{g}} = Q_{\infty,\mathsf{g}} + a' L^{y_1} + w L^{-|2y_t-d|} + \cdots$$

However, we already know

$$Q_{\mathsf{g}} = Q_{\infty,\mathsf{g}} + b L^{y_i} + \cdots$$

Since $y_i \neq -2|y_t - d|$ in general, one *must* have

$$y_1 = -|2y_t - d|$$

as indeed found numerically.

5) Conclusion

- Cluster simulation of new models
- Investigation of constrained systems
- Exploration ‘new’ physics
- Renormalization not OK in canonical ensemble