Graphical Representations and Cluster Algorithms

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Newton Institute, March 27, 2008

Outline

- Introduction to graphical representations and cluster algorithms
- An algorithm for the FK random cluster model ($q>1$)
- Graphical representations and cluster algorithms for Ising systems with external fields and/or frustration

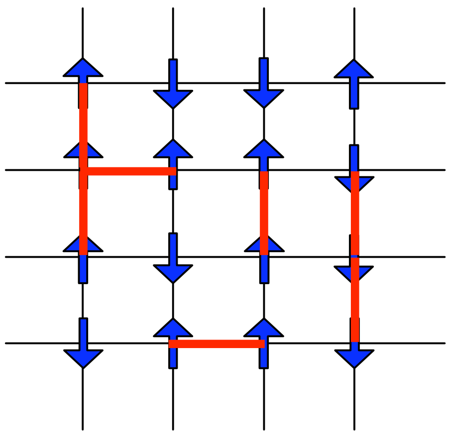
Graphical Representations

- Tool for rigorous results on spin systems
- Basis for very efficient Monte Carlo algorithms
- Source of geometrical insights into phase transitions

Fortuin & Kastelyn
Coniglio & Klein
Swendsen & Wang
Edwards & Sokal

Joint Spin-Bond Distribution

Edwards&Sokal, PRD, **38**,2009 (1988)



$$\mathcal{W}(\sigma,\omega;p) = B_p(\omega)\Delta(\sigma,\omega)$$

$$B_p(\omega) = \prod_{(ij)} p^{\omega_{ij}}(1-p)^{1-\omega_{ij}}$$

Bernoulli factor

$$\sigma_i = \begin{cases} +1 & \uparrow \\ -1 & \downarrow \end{cases}$$

$$\Delta(\sigma,\omega) = \begin{cases} 1 \text{ if for every } (ij)\ \omega_{(ij)} = 1 \rightarrow \sigma_i = \sigma_j \\ 0 \text{ otherwise} \end{cases}$$

$$\omega_{ij} = \begin{cases} 1 \\ 0 \end{cases}$$

Every occupied bond is satisfied

Marginals of ES Distribution

$$\mathcal{W}(\sigma,\omega;p) = B_p(\omega)\Delta(\sigma,\omega)$$

Fortuin-Kastelyn random cluster model for *q=2*

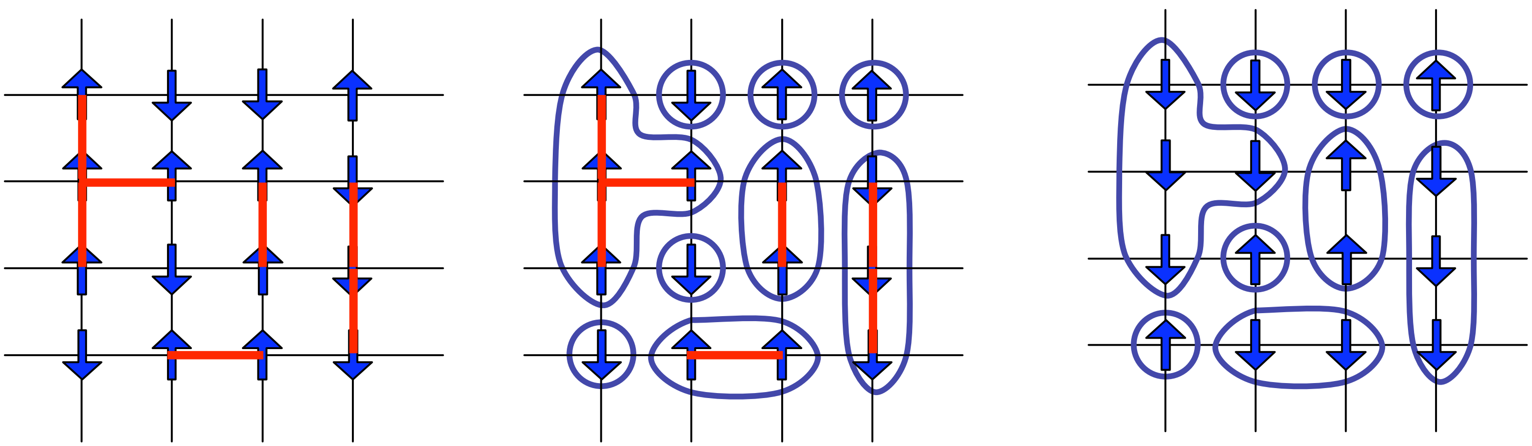
$$\mathcal{W}(\omega;p) = B_p(\omega)2^{\mathcal{C}(\omega)}$$

$\mathcal{C}(\omega)$ *=number of clusters*

Ising model

$$\mathcal{W}(\sigma;p = 1 - e^{-2\beta J}) = e^{\beta J \sum_{(ij)} \sigma_i \sigma_j}$$

Swendsen-Wang Algorithm



- Occupy satisfied bonds with probability $p = 1 - e^{-2\beta J}$
- Identify clusters of occupied bonds
- Randomly flip clusters of spins with probability 1/2.

Connectivity and Correlation

$$\langle \sigma_i \sigma_j \rangle = \mathrm{Prob}\{i \text{ and } j \text{ connected}\}$$

- Broken Symmetry ⟺ Giant cluster

Efficiency at the critical point

- Dynamic Exponent

$$\tau \sim L^z$$

- Li-Sokal bound

$$z \geq \alpha/\nu$$

- L linear dimension
- τ autocorrelation time
- z dynamic exponent
- α specific heat exponent
- ν correlation length exponent

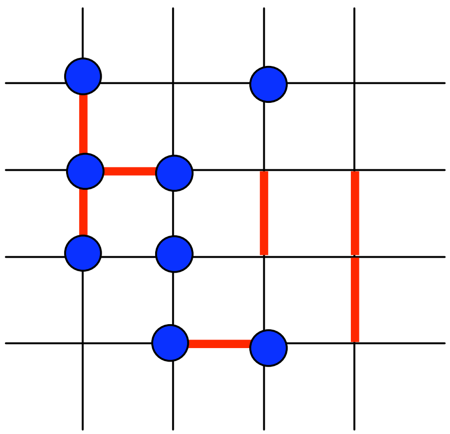
Random cluster model (q>1)

$$\mathcal{W}(\omega; p) = B_p(\omega) q^{\mathcal{C}(\omega)}$$

For q not too large and d>1, there is a continuous phase transition. Above a critical q, the transition is first-order. q=1 is Bernoulli percolation, q=2 is Ising, q=positive integer is Potts.

Edward-Sokal Joint Distribution

L. Chayes & JM, Physica A **254**, 477 (1998)



$$\mathcal{W}(\sigma,\omega;p) = B_p(\omega)(q-1)^{\mathcal{C}(\sigma,\omega)}\Delta(\sigma,\omega)$$

$\mathcal{C}(\sigma,\omega)$ *number of clusters of* ***inactive*** *sites*

$$B_p(\omega) = \prod_{(ij)} p^{\omega_{ij}}(1-p)^{1-\omega_{ij}}$$ *Bernoulli factor*

$$\sigma_i = \begin{cases} 1 \\ 0 \end{cases}$$

$$\Delta(\sigma,\omega) = \begin{cases} 1 \text{ if for every } (ij)\ \omega_{(ij)} = 1 \rightarrow \sigma_i = \sigma_j \\ 0 \text{ otherwise} \end{cases}$$

Every occupied bond is satisfied

$$\omega_{ij} = \begin{cases} 1 \\ 0 \end{cases}$$

Bond marginal is q RC model

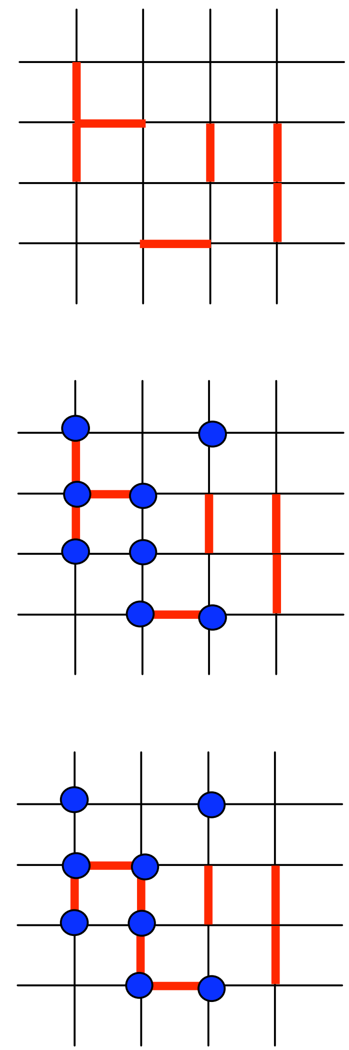
Algorithm for RC model

- Given a bond configuration ω identify clusters
- Declare clusters active with prob $1/q$ and inactive otherwise,

$$\Delta(\sigma,\omega)\left(\frac{1}{q}\right)^{\mathcal{C}(\omega)-\mathcal{C}(\sigma,\omega)}\left(1-\frac{1}{q}\right)^{\mathcal{C}(\sigma,\omega)}$$

- Erase active occupied bonds
- Occupy active bonds with probability p to produce new bond configuration ω',

$$B_p(\omega'_{\text{active}})\Delta(\sigma,\omega')$$



Dynamic Exponent for 2D RC model

Y. Deng, T. M. Garoni, JM, G. Ossola, M. Polin,and A. D. Sokal PRL 99, 055701 (2007)

TABLE I. Dynamic critical exponents $z_{\mathrm{int},\mathcal{E}'}$ for the two-dimensional random-cluster model as a function of q, with preferred fit and minimum L value used in the fit. Error bars are 1 standard deviation, statistical error only. The exact exponents α/ν and β/ν are shown for comparison [22].

q	Fit	$L_{\min}$	$z_{\mathrm{int},\mathcal{E}'}$	α/ν	β/ν
1.00	Exact	...	0	−0.5000	0.1042
1.25	$A + BL^{-p}$	128	0	−0.3553	0.1112
1.50	$A + BL^{-p}$	32	0	−0.2266	0.1168
1.75	$AL^z + B$	16	0.06(1)	−0.1093	0.1213
2.00	$AL^z + B$	32	0.14(1)	0 (log)	0.1250
2.25	$AL^z + B$	32	0.24(1)	0.1036	0.1280
2.50	$AL^z + B$	32	0.31(1)	0.2036	0.1303
2.75	$AL^z + B$	16	0.40(2)	0.3017	0.1321
3.00	$AL^z + B$	32	0.49(1)	0.4000	0.1333
3.25	$AL^z + B$	64	0.57(1)	0.5013	0.1339
3.50	AL^z	16	0.69(1)	0.6101	0.1338
3.75	AL^z	32	0.78(1)	0.7376	0.1324
4.00	$AL^z + B$	32	0.93(2)	1.0000	0.1250

Dynamic Exponent for 3D RC model

TABLE II. Dynamic critical exponents $z_{\text{int},\mathcal{E}'}$ and static exponents α/ν and β/ν for the three-dimensional random-cluster model. For $q = 2$, dynamic data are from Ref. [10] and static exponents are from Ref. [26].

q	Fit	L_{min}	$z_{\text{int},\mathcal{E}'}$	α/ν	β/ν
1.5	AL^z	96	0.13(1)	−0.32(4)	0.500(4)
1.8	AL^z	96	0.29(1)	−0.15(5)	0.5117(6)
2	AL^z	96	0.46(3)	0.174(1)	0.5184(1)
2.2	AL^z	24	0.76(1)	0.50(4)	0.508(4)

Dynamic Exponent for Mean Field RC model

- z=0, 1<q<2,
- z=1, q=2,
- exponential slowing (first-order), q>2
- obtained from an evolution equation for the average size of the largest cluster:

$$m' = \frac{2q-2}{q}m - \frac{4t}{q^2} + \frac{8(q-1)tm}{3q^2} - \frac{2(q-1)^2 m^2}{3q}$$

Conclusions (Part I)

- Swendsen-Wang scheme can be extended to real q>1 RC models.
- Li-Sokal bound not sharp for any q>1

Fields and Frustration

$$\mathcal{H} = -\sum_{(ij)} J_{ij}\sigma_i\sigma_j - \sum h_i\sigma_i$$

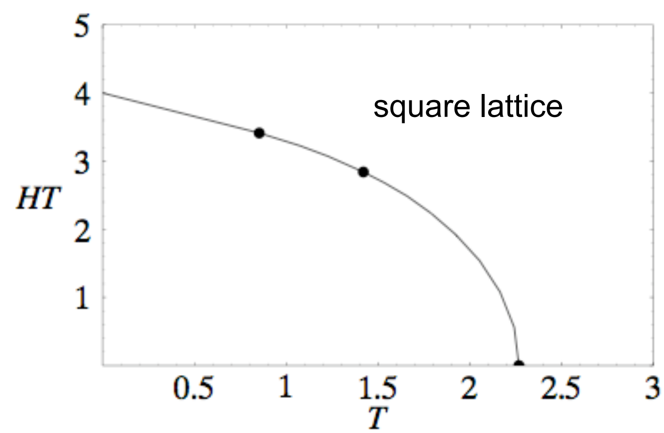
- Ising model in a staggered field
- Spin glass
- Random field Ising model

Ising model in a staggered field
(bipartite lattice)

$$\mathcal{H} = -\sum_{(ij)} J_{ij}\sigma_i\sigma_j - \sum h_i\sigma_i$$

$$J_{ij} = 1$$

$$h_i = \text{parity}(i)H$$



For H not too large and d>1, there is a continuous phase transition in the Ising universality class to a phase with non-zero staggered magnetization

Ising spin glass

$$\mathcal{H} = -\sum_{(ij)} J_{ij}\sigma_i\sigma_j - \sum h_i\sigma_i$$

$$[J_{ij}] = 0$$

frustration%$#@!1

$$[J_{ij}^2] = 1$$

$$h_i = 0$$

i.i.d. quenched disorder

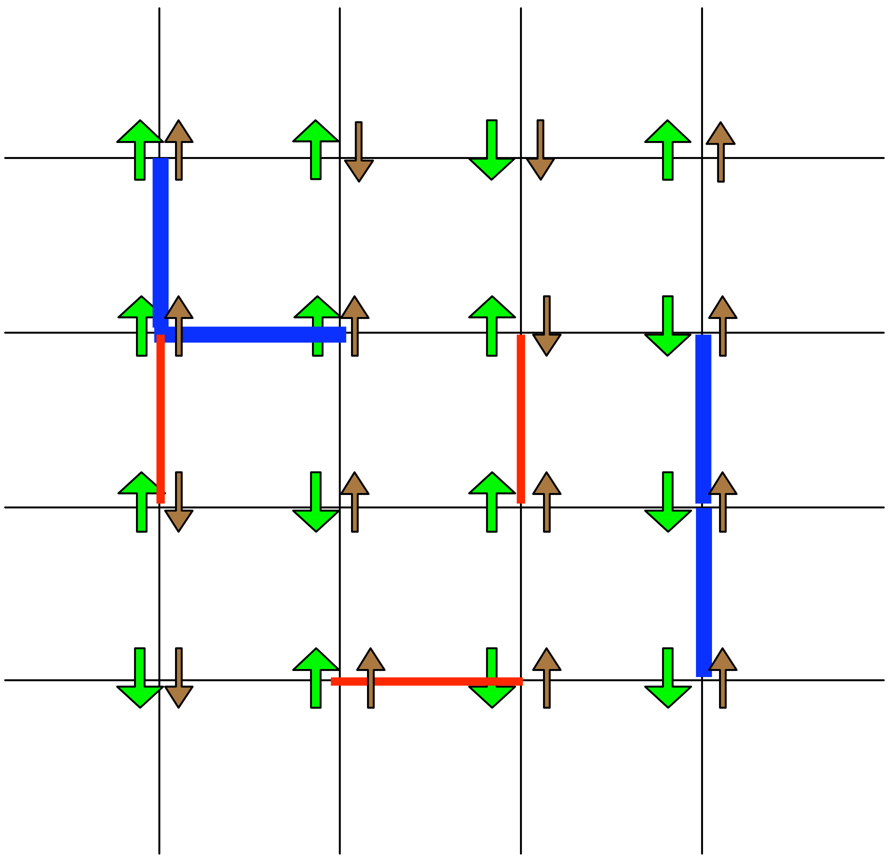
For d>2, there is a continuous phase transition to a state with non-zero Edwards-Anderson order parameter.

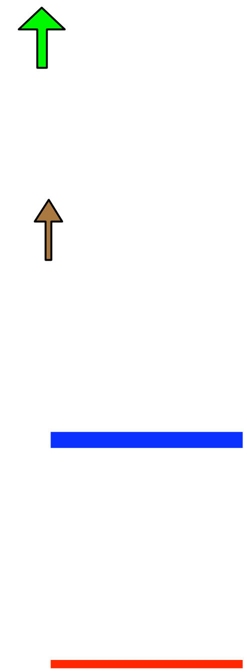
Swendsen-Wang fails with fields or frustration

- No relation between spin correlations and connectivity.
- At T_c one cluster occupies most of the system (e.g. percolation occurs in the high temperature phase).
- External fields h_i cause small acceptance probabilities for cluster flips.

Two Replica Graphical Representation

Swendsen & Wang, PRL, **57**, 2607 (1986) *the other SW paper!*
O. Redner, JM & L. Chayes, PRE **58**, 2749 (1998), JSP **93**, 17 (1998)
JM, M. Newman & L. Chayes, PRE **62**, 8782 (2000)
JM, C. Newman & D. Stein, JSP **130**, 113 (2008)





$\sigma_i = 1$

$\tau_i = 1$

$\omega_{ij} = 1$

$\eta_{ij} = 1$

Spin-Bond Distribution

$$\mathcal{W}(\sigma, \tau, \omega, \eta; \beta, J)$$

$$= B_{2\beta}(\omega) B_\beta(\eta) \Delta(\sigma, \tau, \omega; J) \Gamma(\sigma, \tau, \eta)$$

$$B_\beta(\eta) = \prod_{(ij)} (1 - e^{-2\beta})^{\eta_{ij}} (e^{-2\beta})^{1-\eta_{ij}}$$

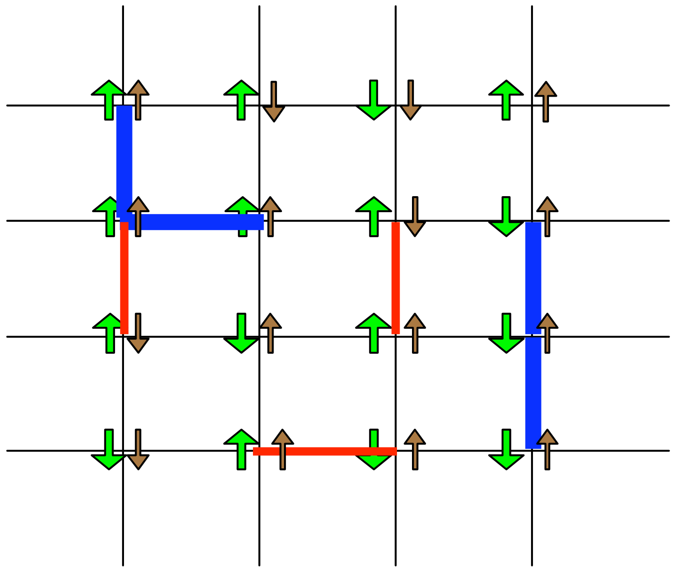
Bernoulli factor

$$\Delta(\sigma, \tau, \omega; J) = \begin{cases} 1 \text{ if for every } (ij)\ \omega_{ij} = 1 \rightarrow J_{ij}\sigma_i\sigma_j > 0 \text{ and } J_{ij}\tau_i\tau_j > 0 \\ 0 \text{ otherwise} \end{cases}$$

$$\Gamma(\sigma, \tau, \eta) = \begin{cases} 1 \text{ if for every } (ij)\ \eta_{ij} = 1 \rightarrow \sigma_i\sigma_j\tau_i\tau_j < 0 \\ 0 \text{ otherwise} \end{cases}$$

spin bond constraints

Spin Bond Constraints



•If bonds satisfied in *both* replicas then

$$\omega_{ij} = 1$$

with probability $p = 1 - e^{-4\beta}$

•If bonds satisfied in only *one* replica then

$$\eta_{ij} = 1$$

with probability $p = 1 - e^{-2\beta}$

Properties

- Spin marginal is two independent Ising systems

$$\mathcal{W}_{\text{spin}}(\sigma,\tau;\beta,J) = \text{const} \times \exp\left[\beta \sum_{(ij)} J_{ij}(\sigma_i\sigma_j + \tau_i\tau_j)\right]$$

- Correlation function of EA order parameter and connectivity

$$\langle \sigma_i \tau_i \sigma_j \tau_j \rangle =$$

Prob{ *i* and *j* are connected by a path of occupied bonds with an **even** number of red bonds}

–

Prob{ *i* and *j* are connected by a path of occupied bonds with an **odd** number of red bonds}

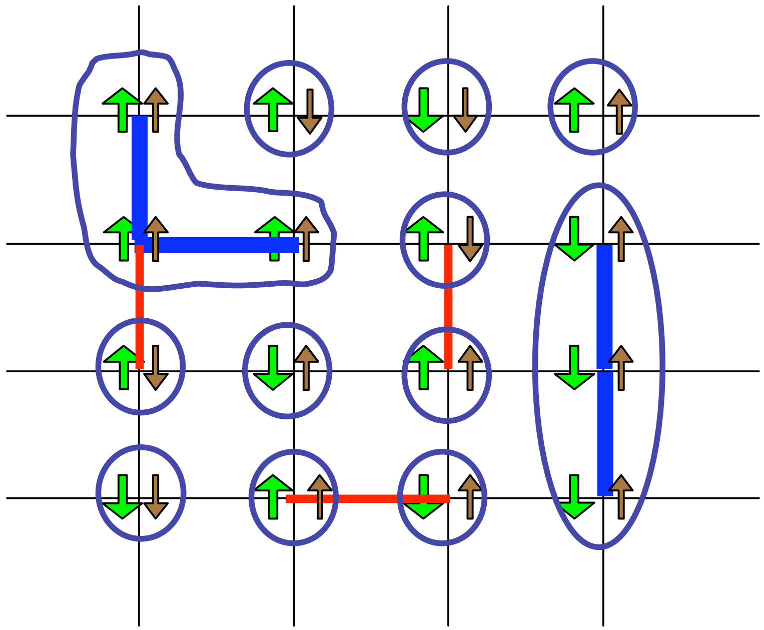
Properties II

- For ferromagnetic Ising systems, including the staggered field and random field Ising models, percolation of blue bonds is equivalent to broken symmetry.

- For Ising systems with AF interactions, the existence of a blue cluster with a density strictly larger than all other blue cluster is equivalent to broken symmetry.

Two Replica Cluster Algorithm

- Given a two spin configurations
- Occupy bonds
- Identify clusters

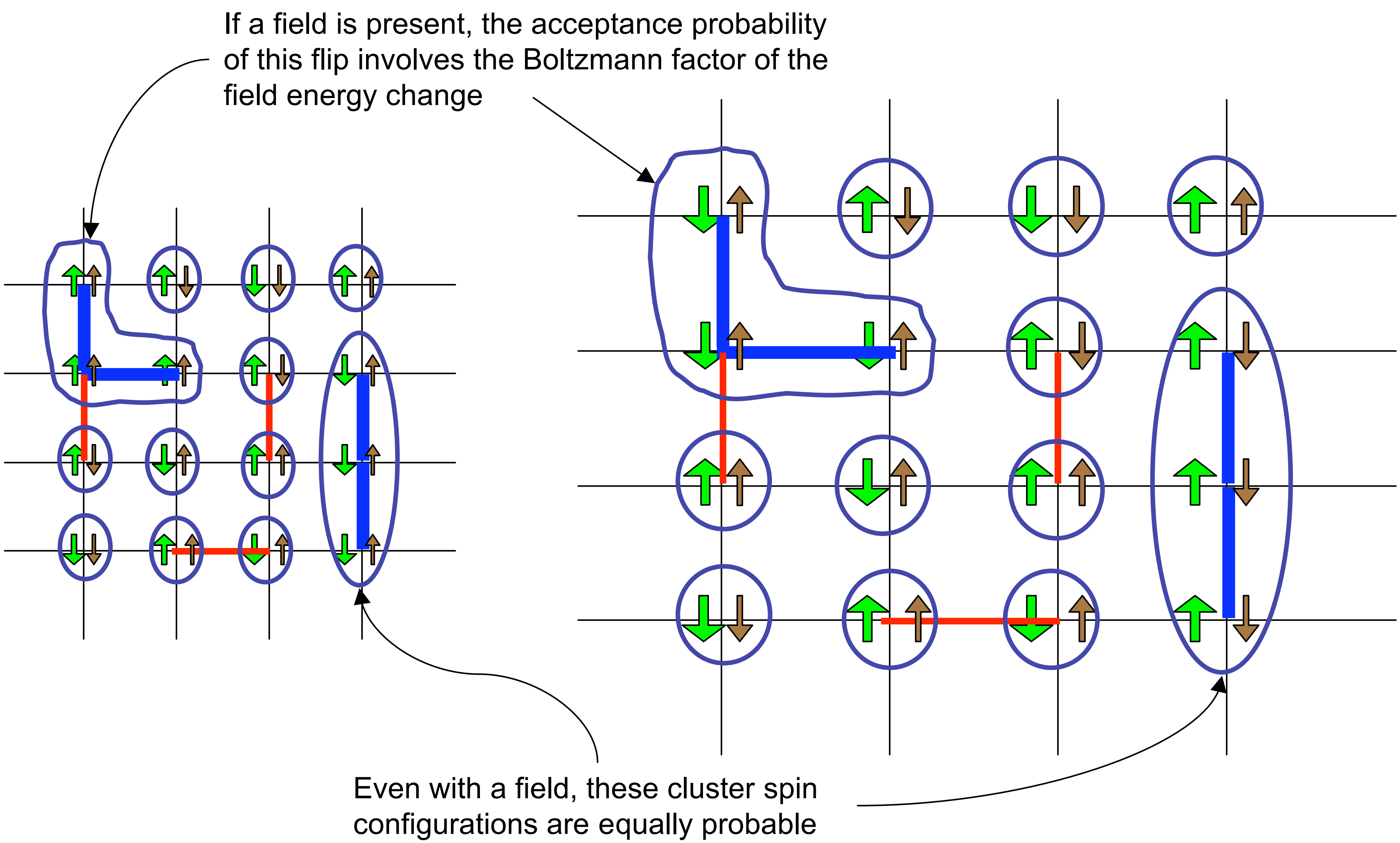


$$p = 1 - e^{-4\beta}$$

$$p = 1 - e^{-2\beta}$$

For purposes of this example, assume all bonds FM

Re-populate spins consistent with constraints



Two Replica Cluster Algorithm

- Given two spin configurations in the same environment.
- Blue (red) **occupy** doubly (singly) **satisfied bonds**.
- **Identify** blue and red **clusters**.
- Re-populate spins with equal probability consistent with constraints due to bonds (**flip clusters**).
- **Erase** blue and red **bonds**.
- Add-ons:
  - Translations and global flips of replicas relative to each other (staggered field, bipartite lattice only)
  - Metropolis sweeps
  - Parallel tempering

How well does it work?

2D Ising model in a staggered field

TABLE III: Magnetization integrated autocorrelation times and CPU times for several algorithms for $L = 80$.

X. Li & JM, Int. J. Mod. Phys. C**12**, 257 (2001)

Algorithm	Integrated Autocorrelation Time			CPU time
	$H = 0$	$H = 2$	$H = 4$	(10^{-6} sec/sweep/spin)
TRC	37.3 ± 0.6	39.8 ± 0.7	40.4 ± 0.8	3.1
TRC odd translations only	46 ± 1	54 ± 2	55 ± 1	3.0
TRC even translations only	186 ± 18	283 ± 27	435 ± 43	2.9
TRC & inactive flips even translations only	33.6 ± 0.9	246 ± 27	372 ± 23	4.6
TRC no translations	335 ± 18	440 ± 24	773 ± 47	2.6
Swendsen-Wang	4.12 ± 0.02	4682 ± 173	5707 ± 48	1.3
Metropolis	928 ± 99	1892 ± 158	2959 ± 236	1.1

$z<0.5$

2D Spin Glass

J. S. Wang & R. H. Swendsen, Prog. Theor. Phys. Suppl, vol 157, 317 (2005)

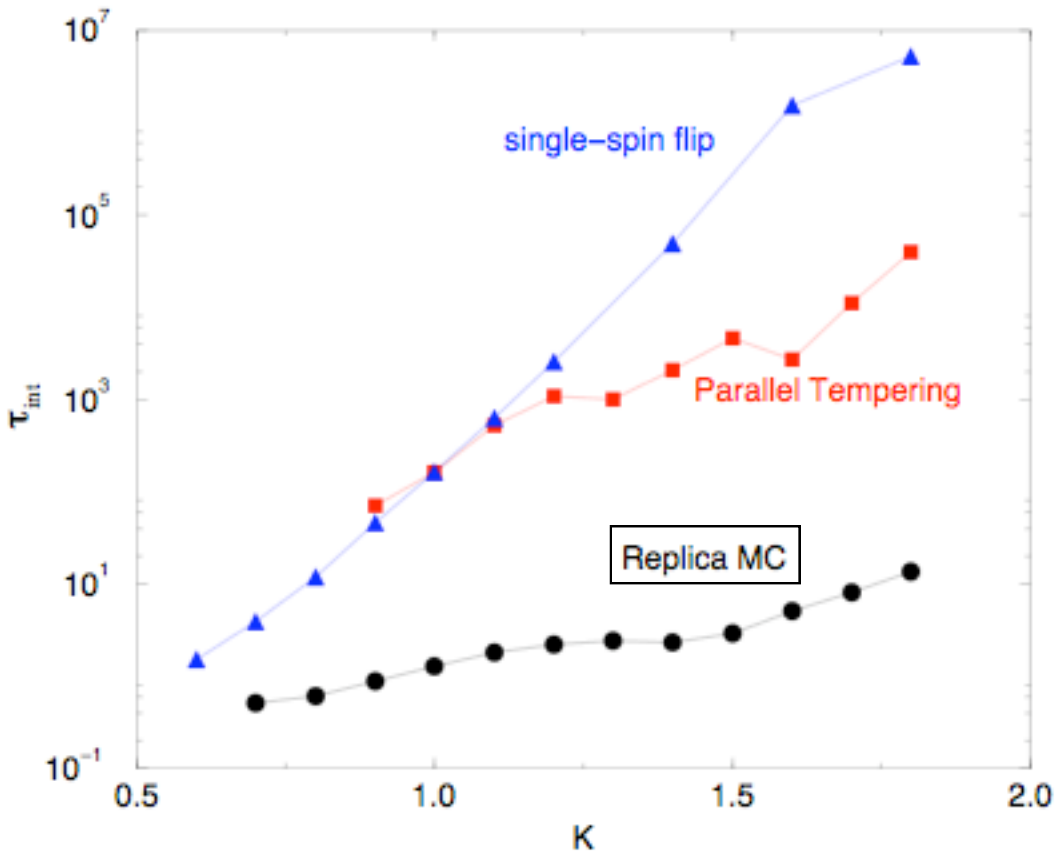
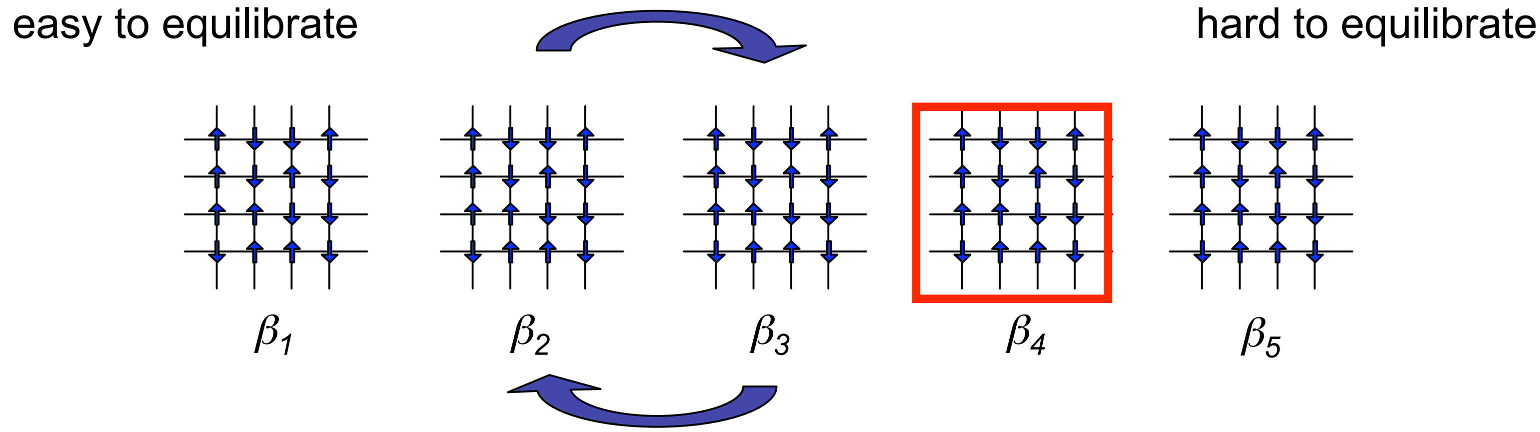


Fig. 2. Comparison of integrated correlation time on a 128 × 128 lattice for single-spin-flip (triangles), parallel tempering (squares), and replica Monte Carlo (circles). The $K = \beta J$ value is distributed from 0.1 to 1.8 in spacing of 0.1. Typically, 10^6 MCS are used.

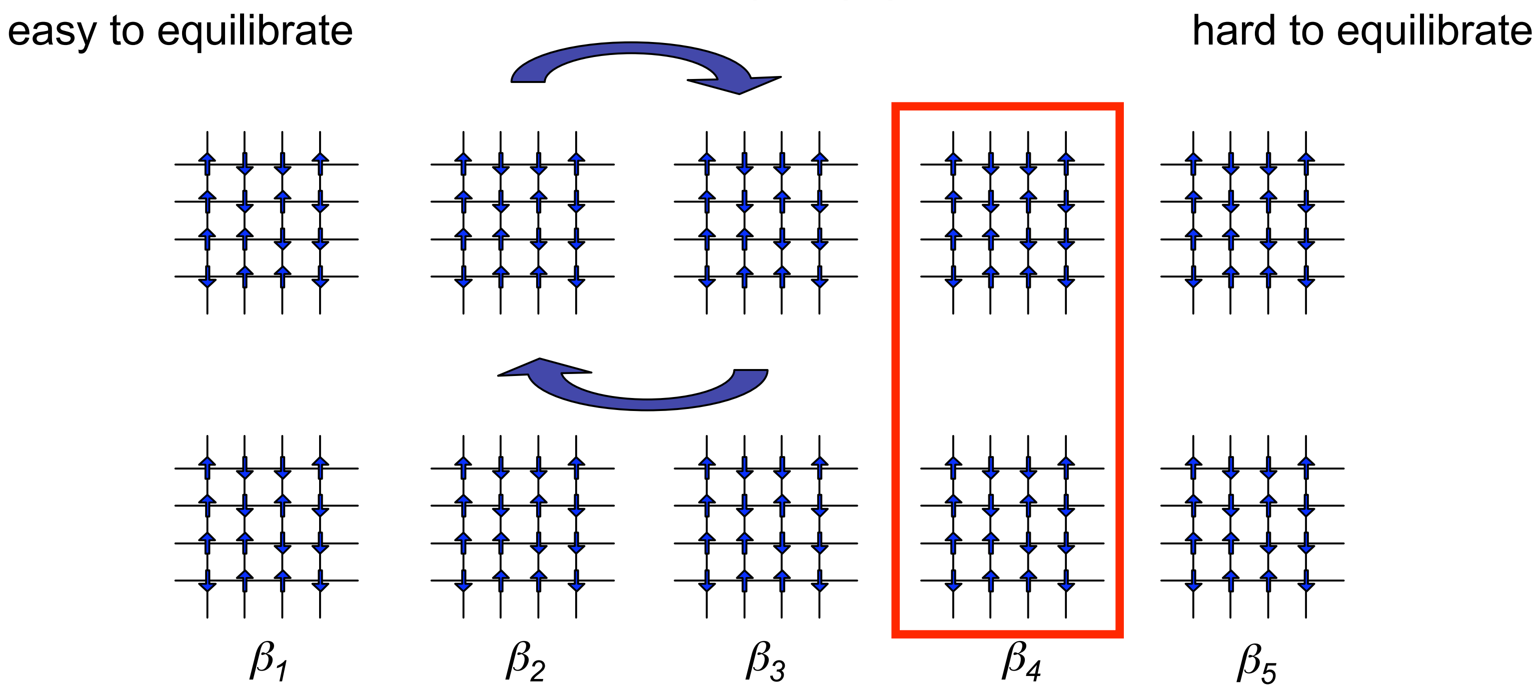
Parallel Tempering



- n replicas at temperatures $\beta_1 \ldots \beta_n$
- MC (e.g. Metropolis) on each replica
- Exchange replicas with energies E and E' and temperatures β and β', with probability:

$$\min\{\exp[(\beta - \beta')(E - E')],1\}$$

Parallel Tempering+Two Replica Cluster Moves



- n replicas at temperatures $\beta_1 \ldots \beta_n$
- Two replica cluster moves at each temperature
- Exchange replicas.

Diluted 3D spin glass

T. Jorg, Phys. Rev. B 73, 224431 (2006)

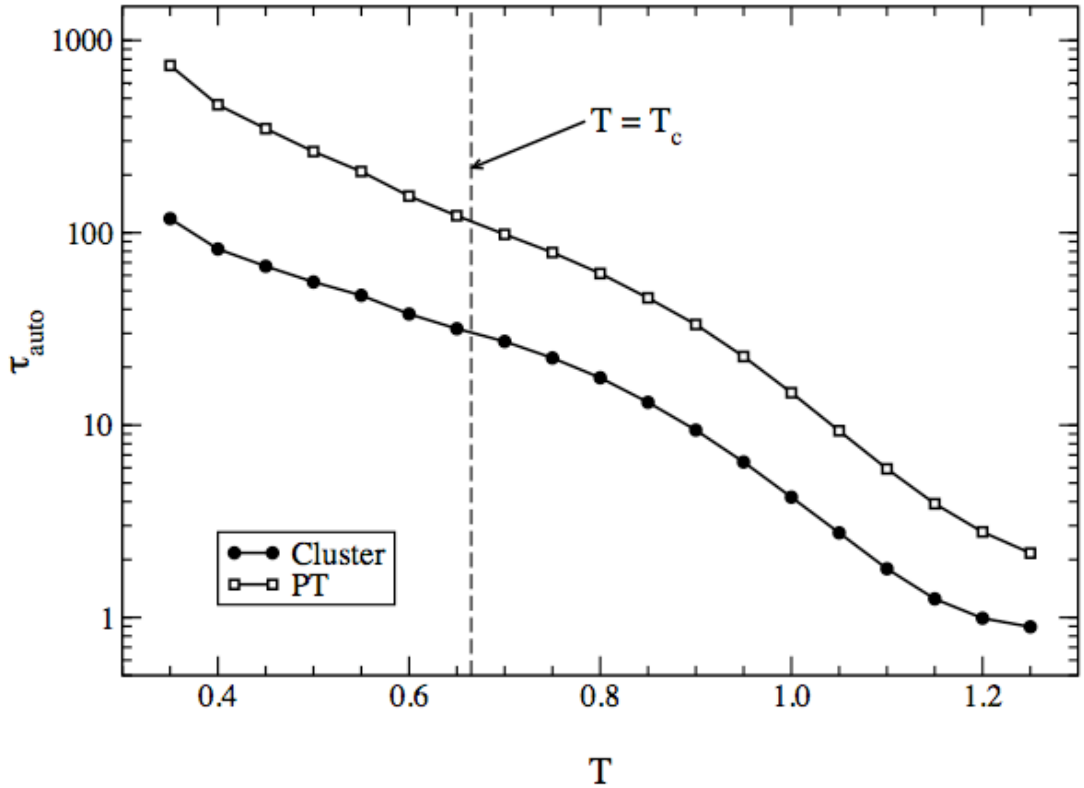


FIG. 1: Qualitative comparison of the integrated autocorrelation time $\tau_{\rm auto}$ as a function of temperature between parallel tempering (PT) and the replica cluster algorithm (Cluster) averaged on the same 20 configurations at $L = 10$.

3D Spin Glass

- For the $d>2$ spin glasses, two giant clusters ("agree" and "disagree" spins) appear in the high temperature phase and together comprise most of the system.
- The signature of the spin glass transition is the onset of a density difference between the two giant clusters.
- The algorithm is not much more efficient that parallel tempering alone.

JM, C. Newman & D. Stein, JSP **130**, 113 (2008)

Conclusions (Part II)

- The two-replica graphical representation and associated algorithms are promising approaches for spin systems with fields or frustration.

However…

- For the hardest systems, e.g. 3D Ising spin glass,the algorithm is not much more efficient than parallel tempering.