# 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

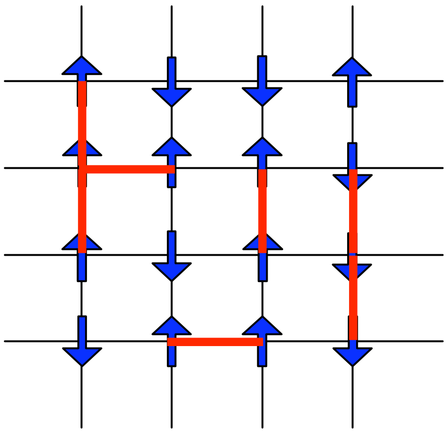
•Basis for very efficient Monte Carlo algorithms

•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*

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

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



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

*Every occupied bond is satisfied*

# Marginals of ES Distribution

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

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

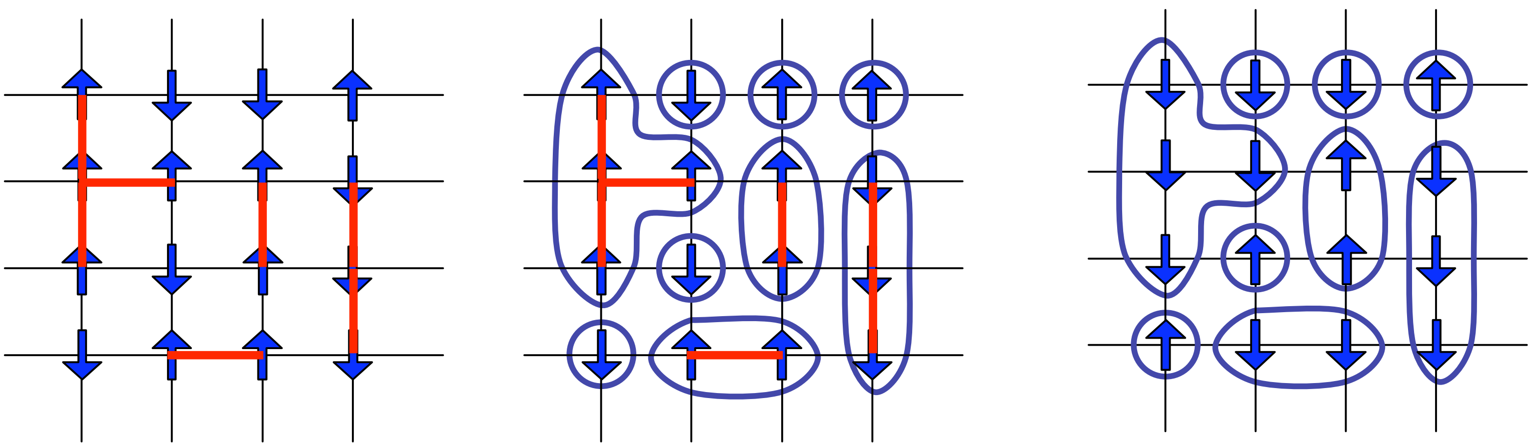
$$\mathcal{W}(\omega;p) = B_p(\omega)2^{\mathcal{C}(\omega)}$$

$\mathcal{C}(\omega)$ *=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
- $\tau$ autocorrelation time
- $z$ dynamic exponent
- $\alpha$ specific heat exponent
- $\nu$ correlation length exponent

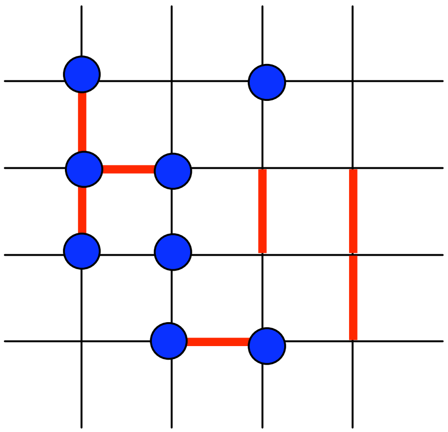
# Random cluster model ($q$>1)

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

*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)

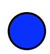


$$\mathcal{W}(\sigma,\omega;p) = B_p(\omega)(q-1)^{\mathcal{C}(\sigma,\omega)}\Delta(\sigma,\omega)$$

$\mathcal{C}(\sigma,\omega)$ *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

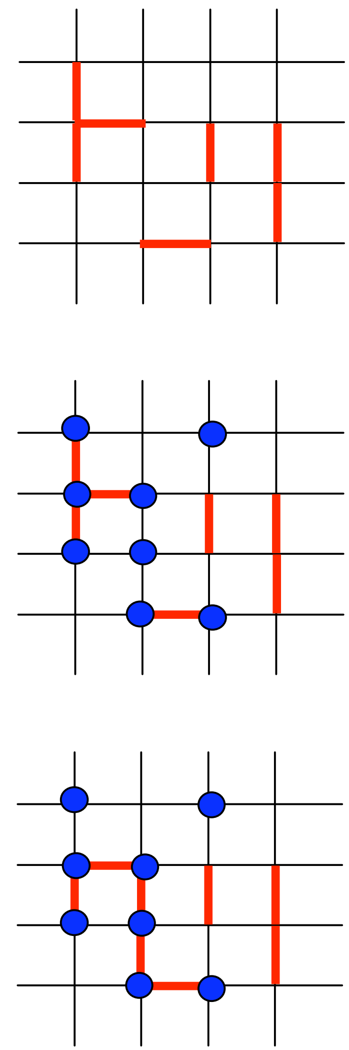
# Algorithm for RC model

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

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

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

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



# 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 $\alpha/\nu$ and $\beta/\nu$ are shown for comparison [22].

| $q$ | Fit | $L_{\mathrm{min}}$ | $z_{\mathrm{int},\mathcal{E}'}$ | $\alpha/\nu$ | $\beta/\nu$ |
|---|---|---|---|---|---|
| 1.00 | Exact | $\cdots$ | 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 $\alpha/\nu$ and $\beta/\nu$ 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 | $L_{\min}$ | $z_{\text{int},\mathcal{E}'}$ | $\alpha/\nu$ | $\beta/\nu$ |
|---|---|---|---|---|---|
| 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

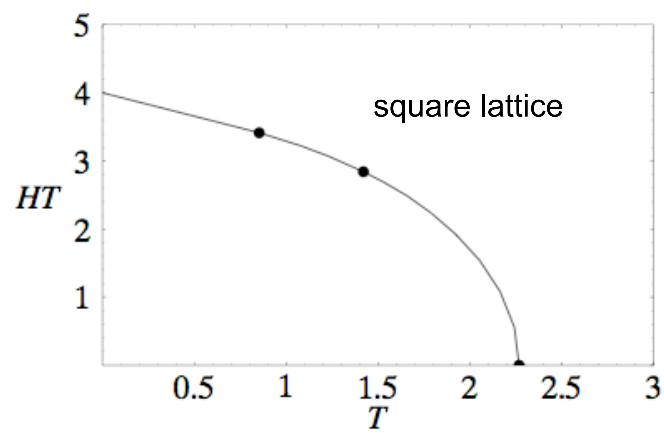
# Ising model in a staggered field

# (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

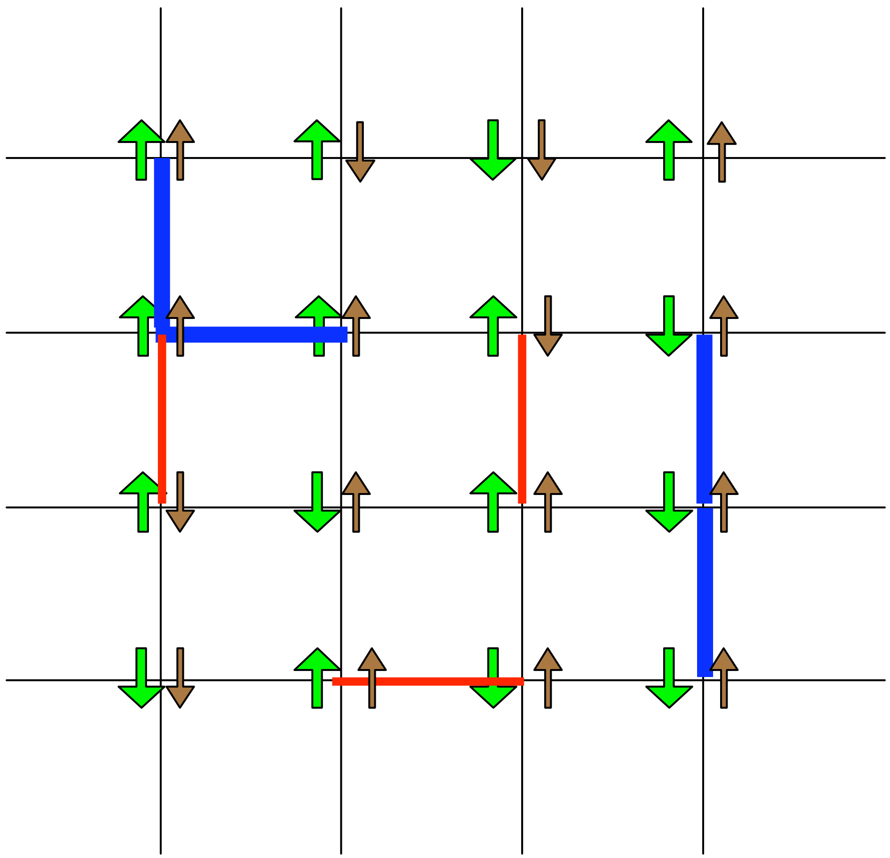
*For d>2, there is a continuous phase transition to a state with non-zero Edwards-Anderson order parameter.*

# 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

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

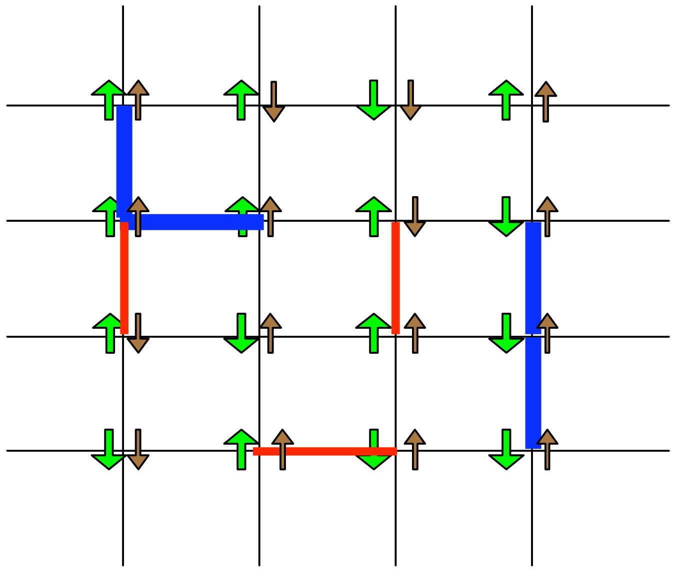
$$B_\beta(\eta) = \prod_{(ij)}(1-e^{-2\beta})^{\eta_{ij}}(e^{-2\beta})^{1-\eta_{ij}}$$ Bernoulli factor

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

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

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}

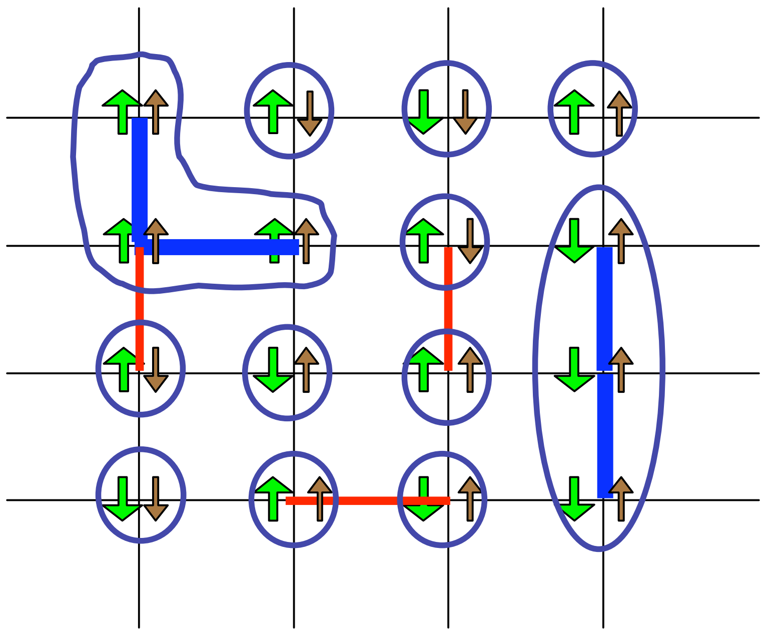
# Properties II

- 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

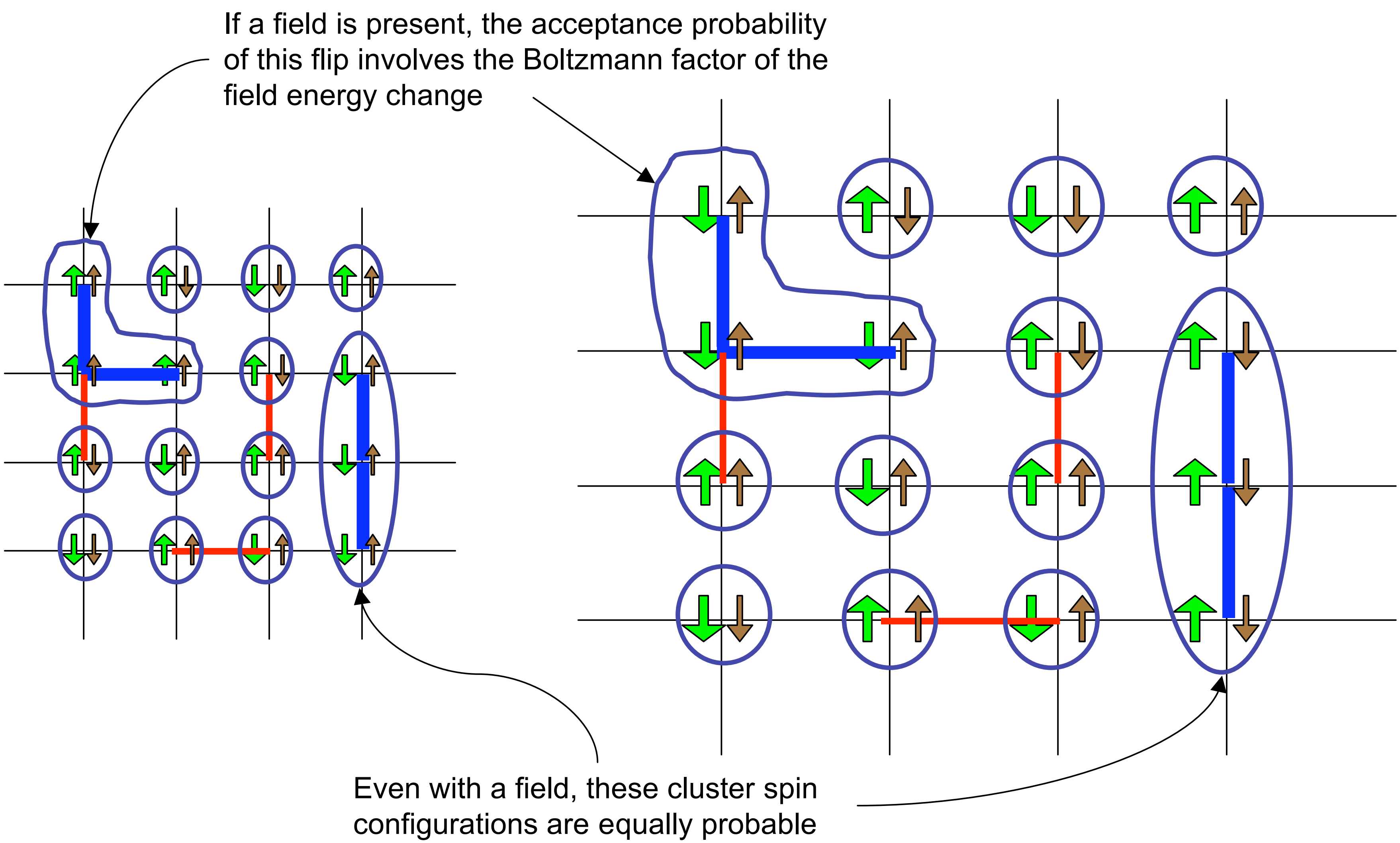


$$p = 1 - e^{-4\beta}$$

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

*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 | $37.3 \pm 0.6$ | $39.8 \pm 0.7$ | $40.4 \pm 0.8$ | 3.1 |
| TRC odd translations only | $46 \pm 1$ | $54 \pm 2$ | $55 \pm 1$ | 3.0 |
| TRC even translations only | $186 \pm 18$ | $283 \pm 27$ | $435 \pm 43$ | 2.9 |
| TRC & inactive flips even translations only | $33.6 \pm 0.9$ | $246 \pm 27$ | $372 \pm 23$ | 4.6 |
| TRC no translations | $335 \pm 18$ | $440 \pm 24$ | $773 \pm 47$ | 2.6 |
| Swendsen-Wang | $4.12 \pm 0.02$ | $4682 \pm 173$ | $5707 \pm 48$ | 1.3 |
| Metropolis | $928 \pm 99$ | $1892 \pm 158$ | $2959 \pm 236$ | 1.1 |

$z<0.5$

# 2D Spin Glass

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

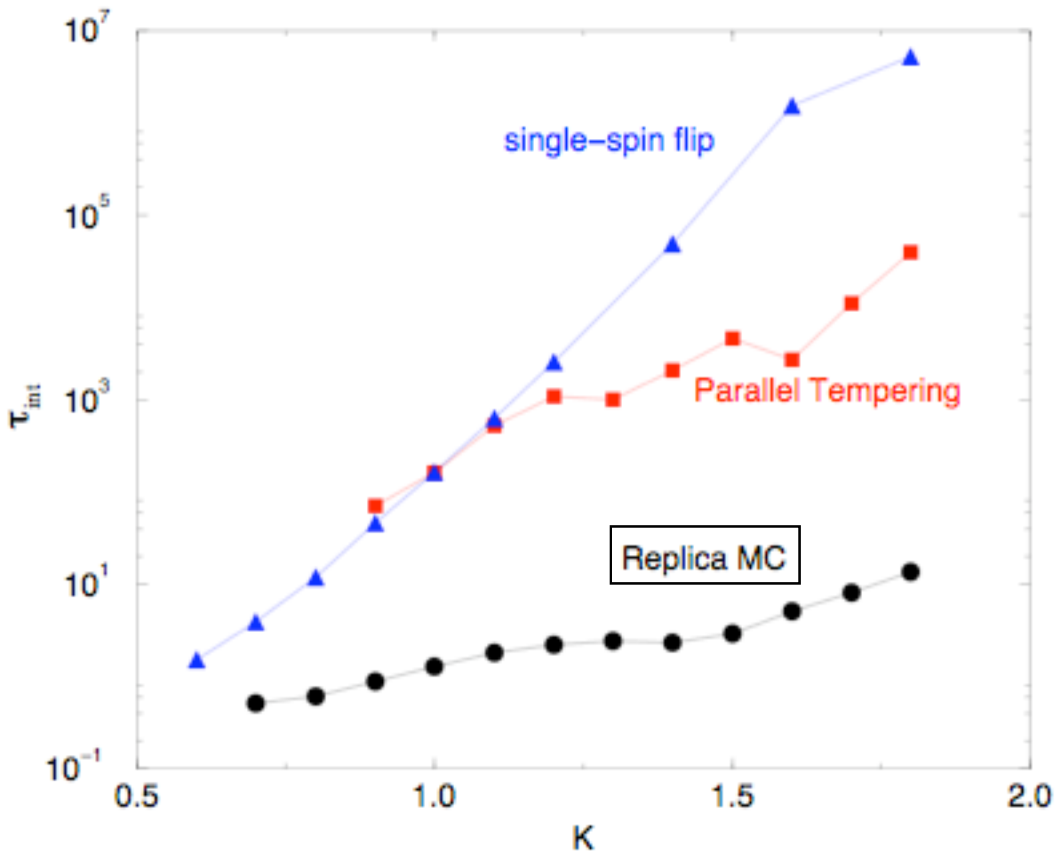
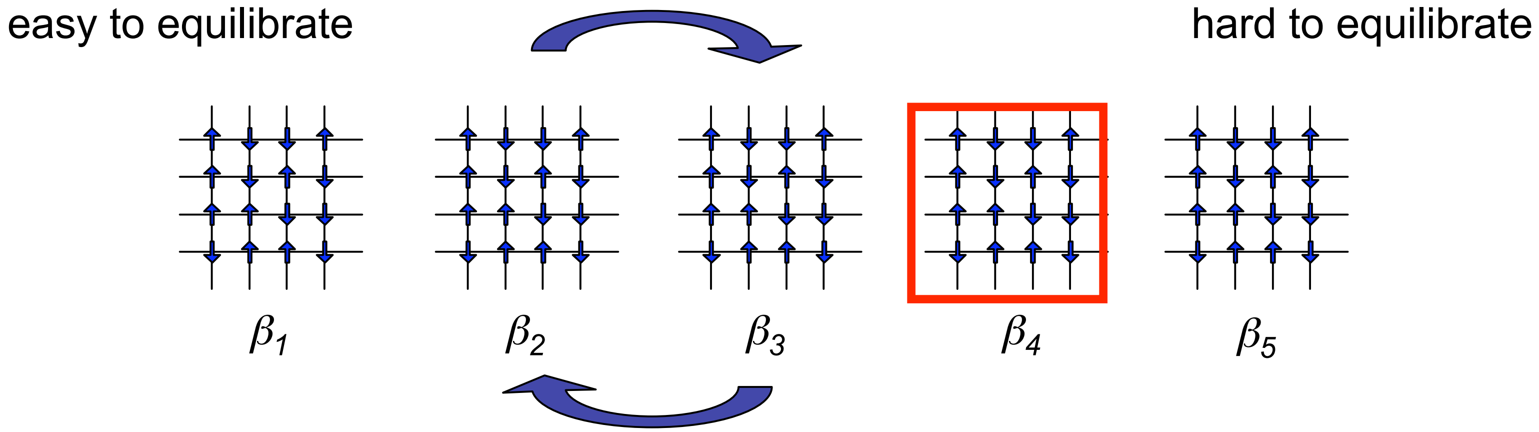



Fig. 2. Comparison of integrated correlation time on a 128 × 128 lattice for single-spin-flip (triangles), parallel tempering (squares), and replica Monte Carlo (circles). The $K = \beta J$ value is distributed from 0.1 to 1.8 in spacing of 0.1. Typically, $10^6$ MCS are used.

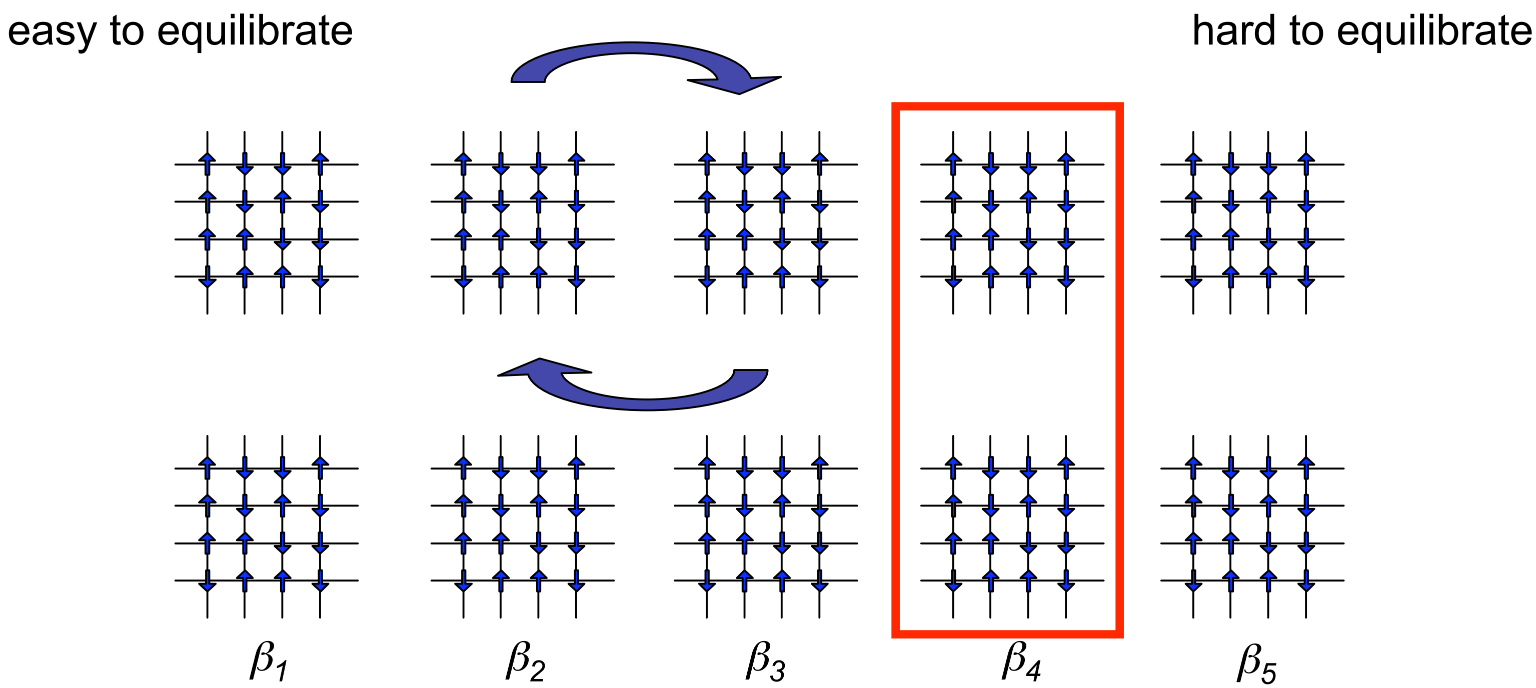
# Parallel Tempering




- *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 $\beta$ and $\beta'$, 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)

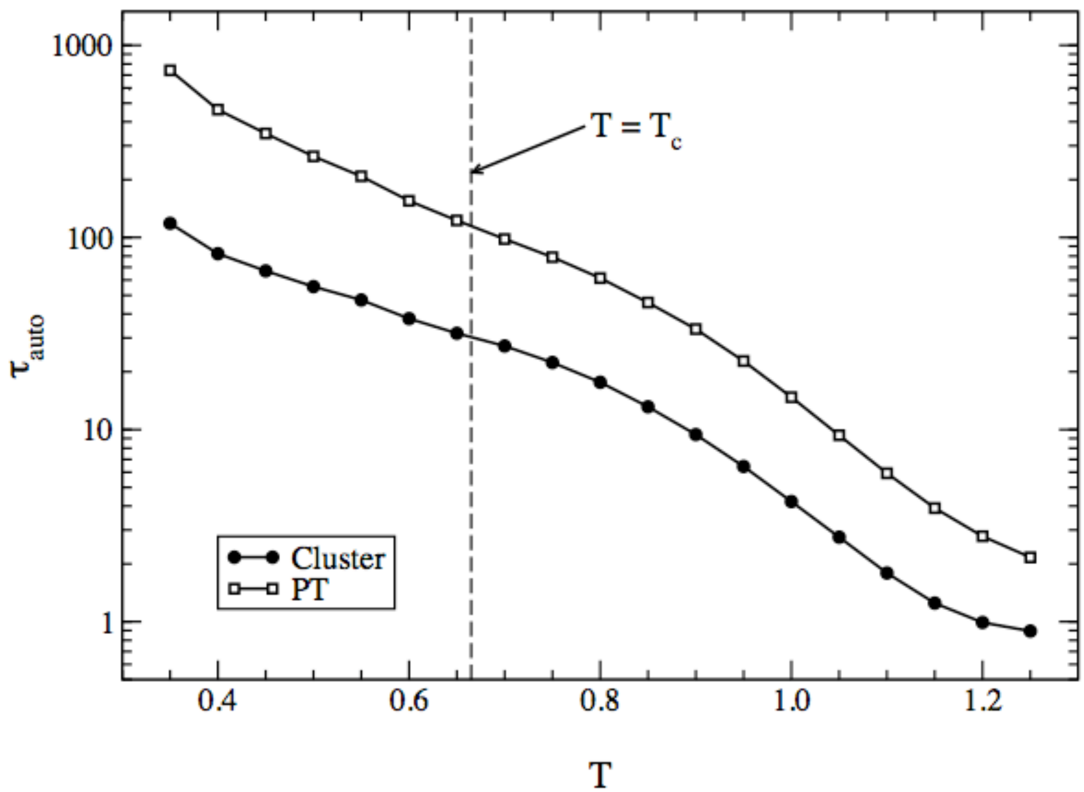



FIG. 1: Qualitative comparison of the integrated autocorrelation time $\tau_{\rm auto}$ as a function of temperature between parallel tempering (PT) and the replica cluster algorithm (Cluster) averaged on the same 20 configurations at $L = 10$.

# 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.