Parallel Tempering Monte Carlo & Spin Glasses

Bradley Dice

Dec. 8, 2016

Ising Model

- Standard approaches use…
  - a fixed temperature
  - a coupling constant J that is constant over the grid

Spin Glasses

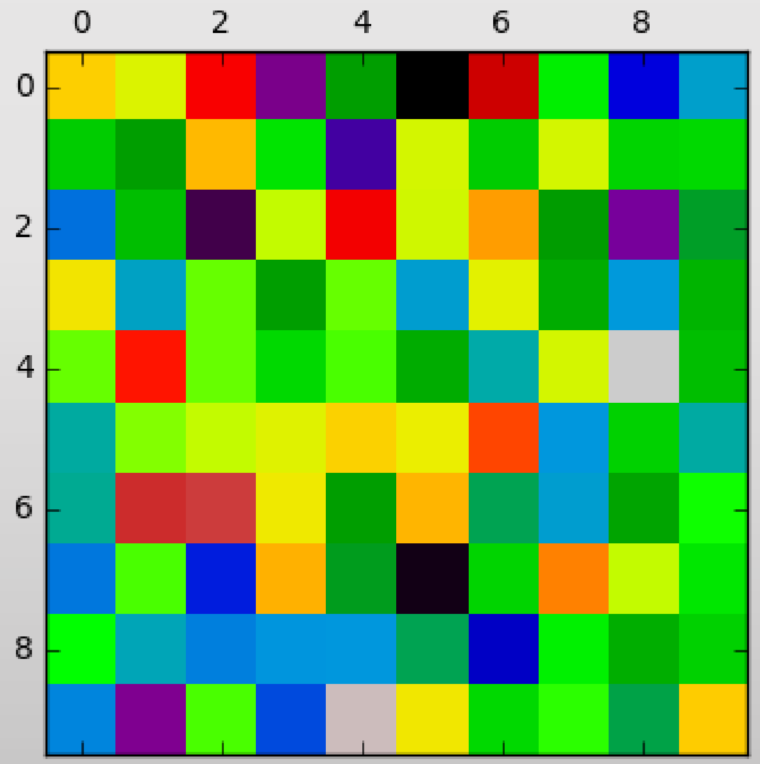
$$\mathrm{H} = -\sum_{<i,j>} J_{ij} S_i S_j$$

- Edwards-Anderson Model
- Each neighboring pair shares a “bond” as before
- Bond couplings J_{ij} are drawn from a normal distribution with $\mu = 0, \sigma = 1$
- Sometimes neighbors want to align…

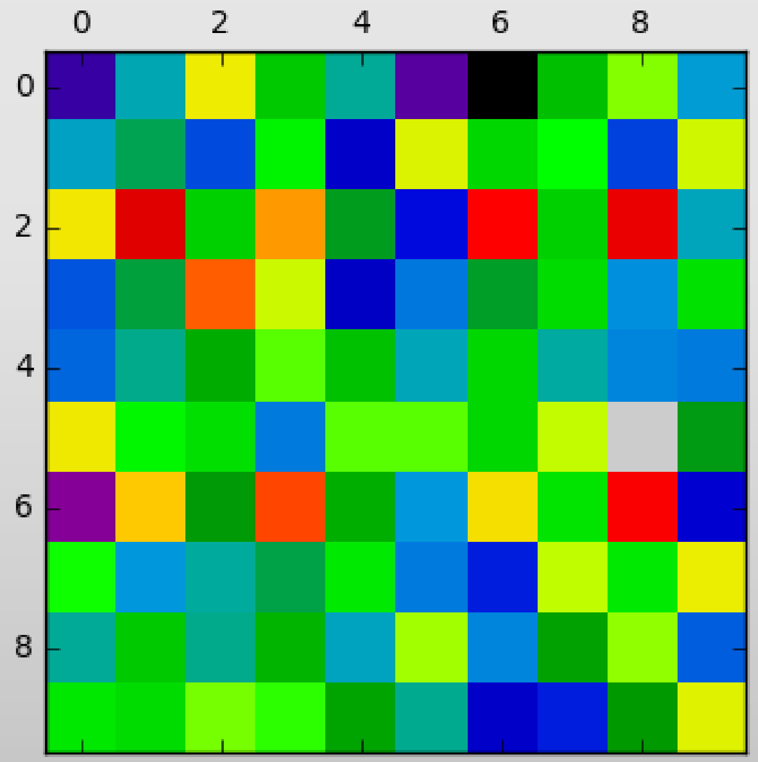
  … and sometimes they want to anti-align.

Bond couplings J_{ij}, 2D

Couplings along x

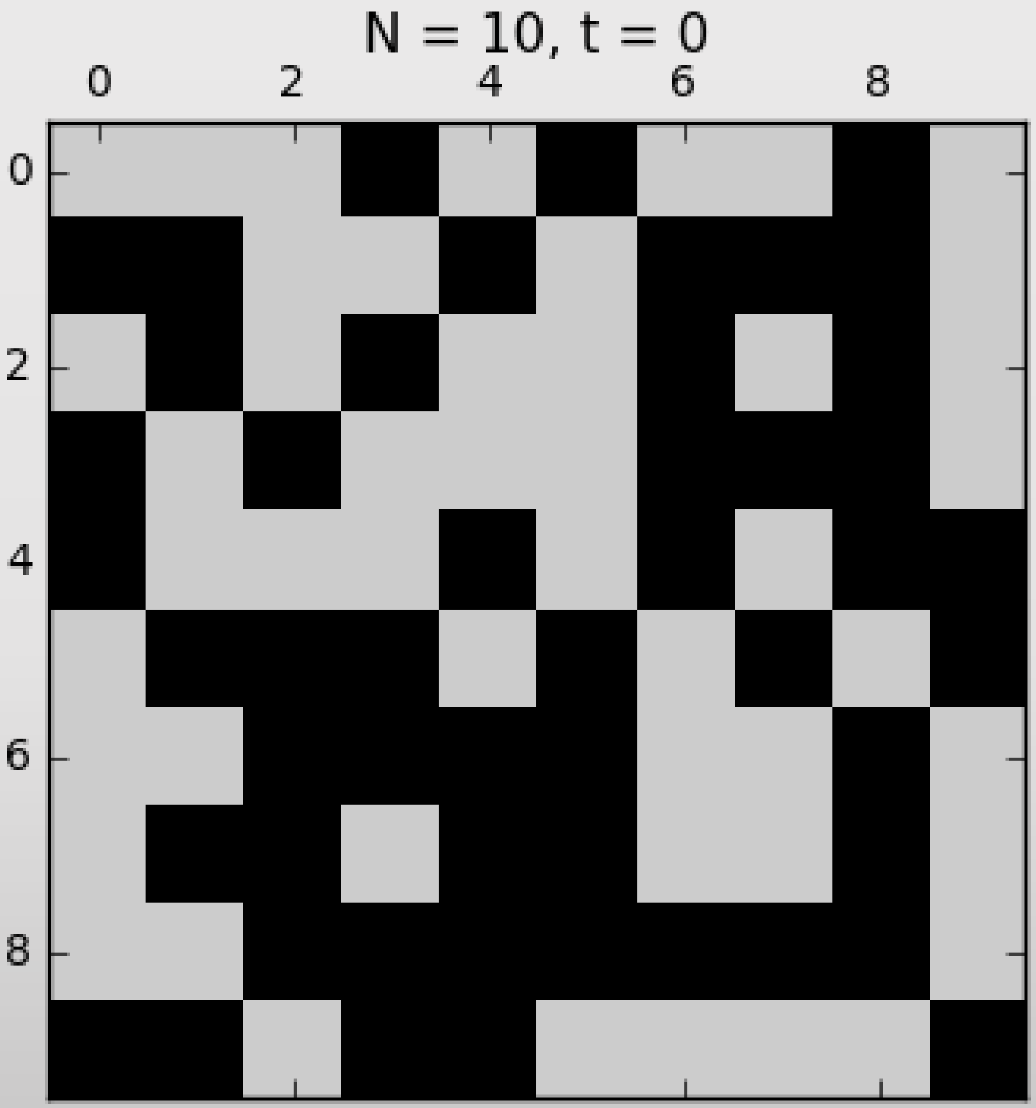


Couplings along y



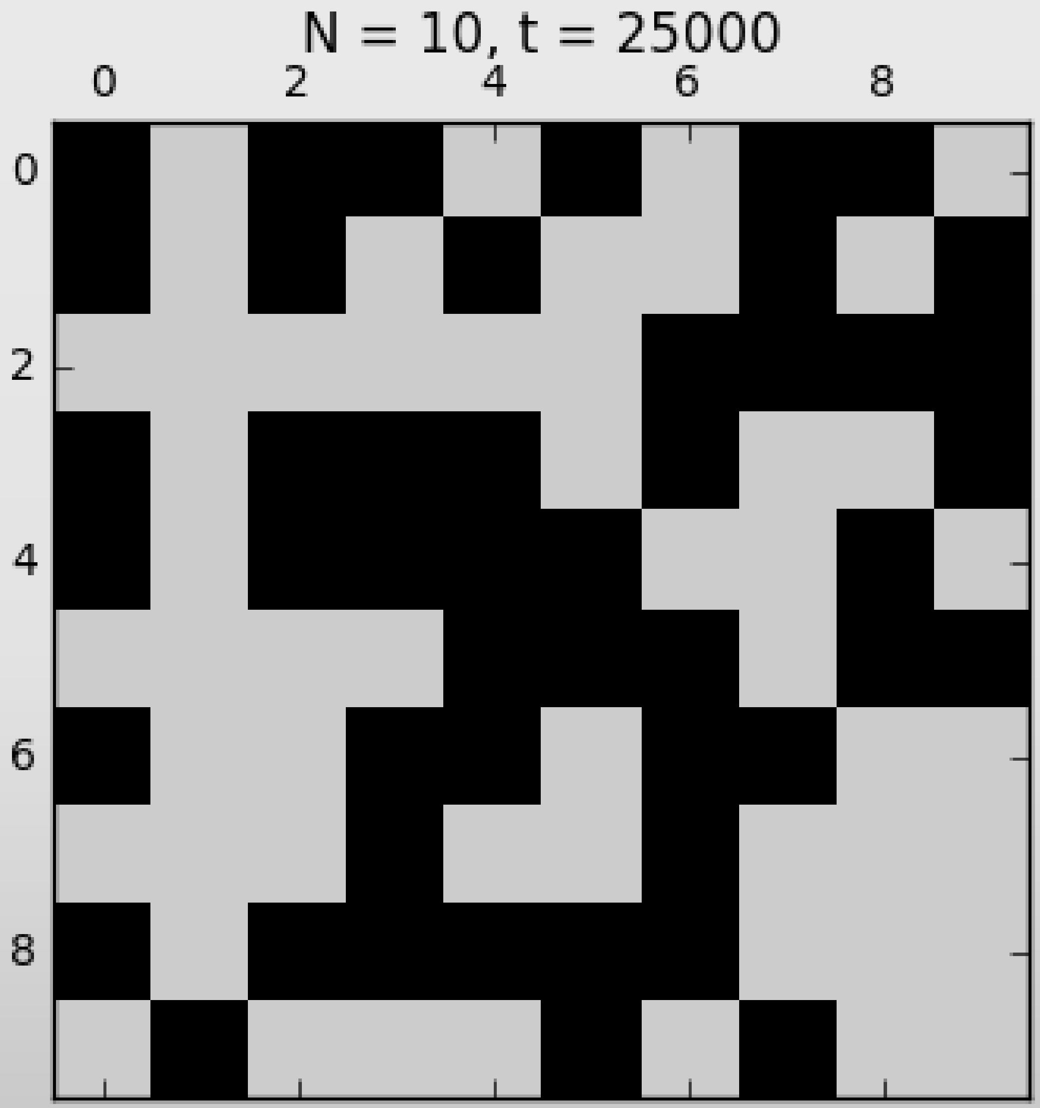
Sample 2D Spin Glass

$$kT = 0.5$$



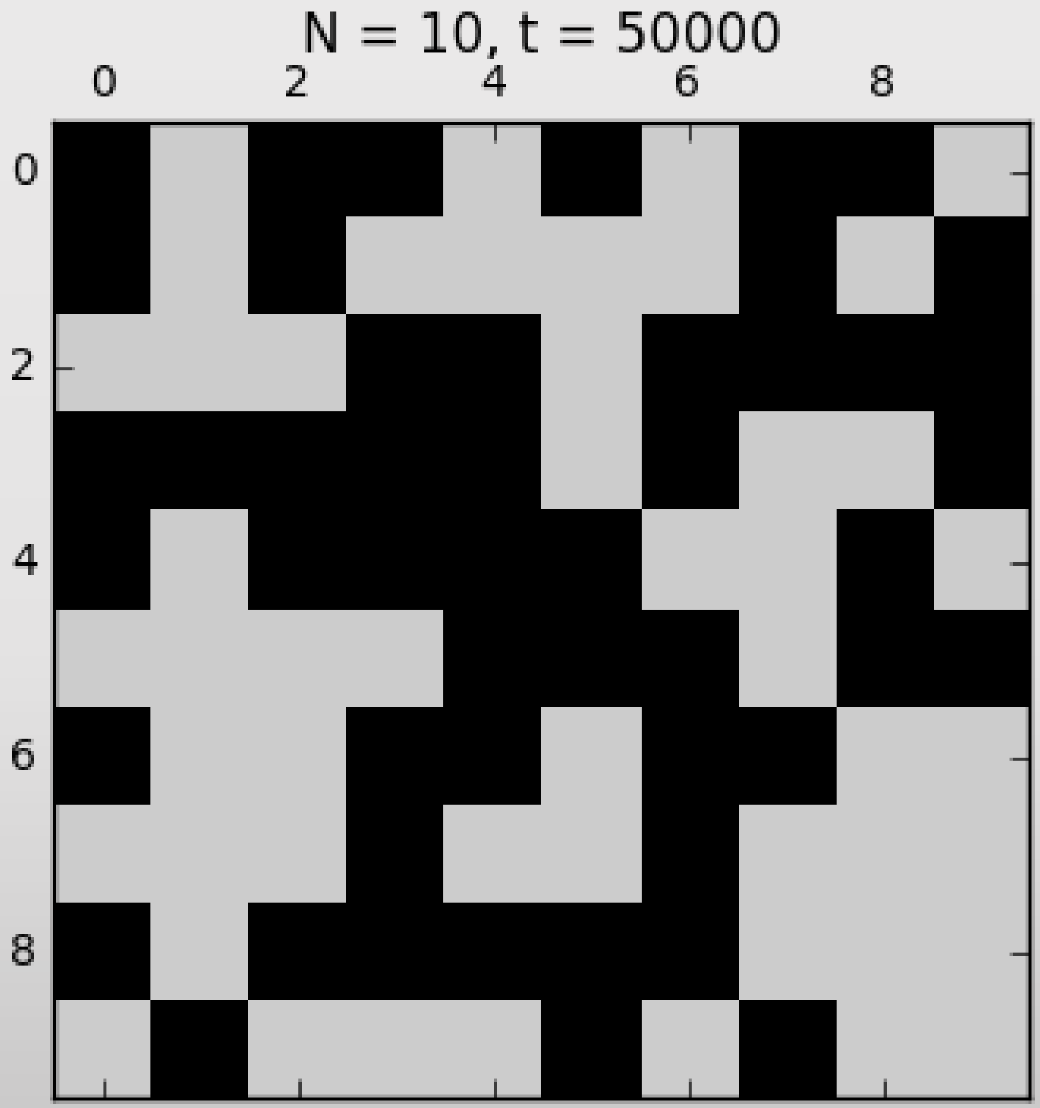
Sample 2D Spin Glass

$$kT = 0.5$$



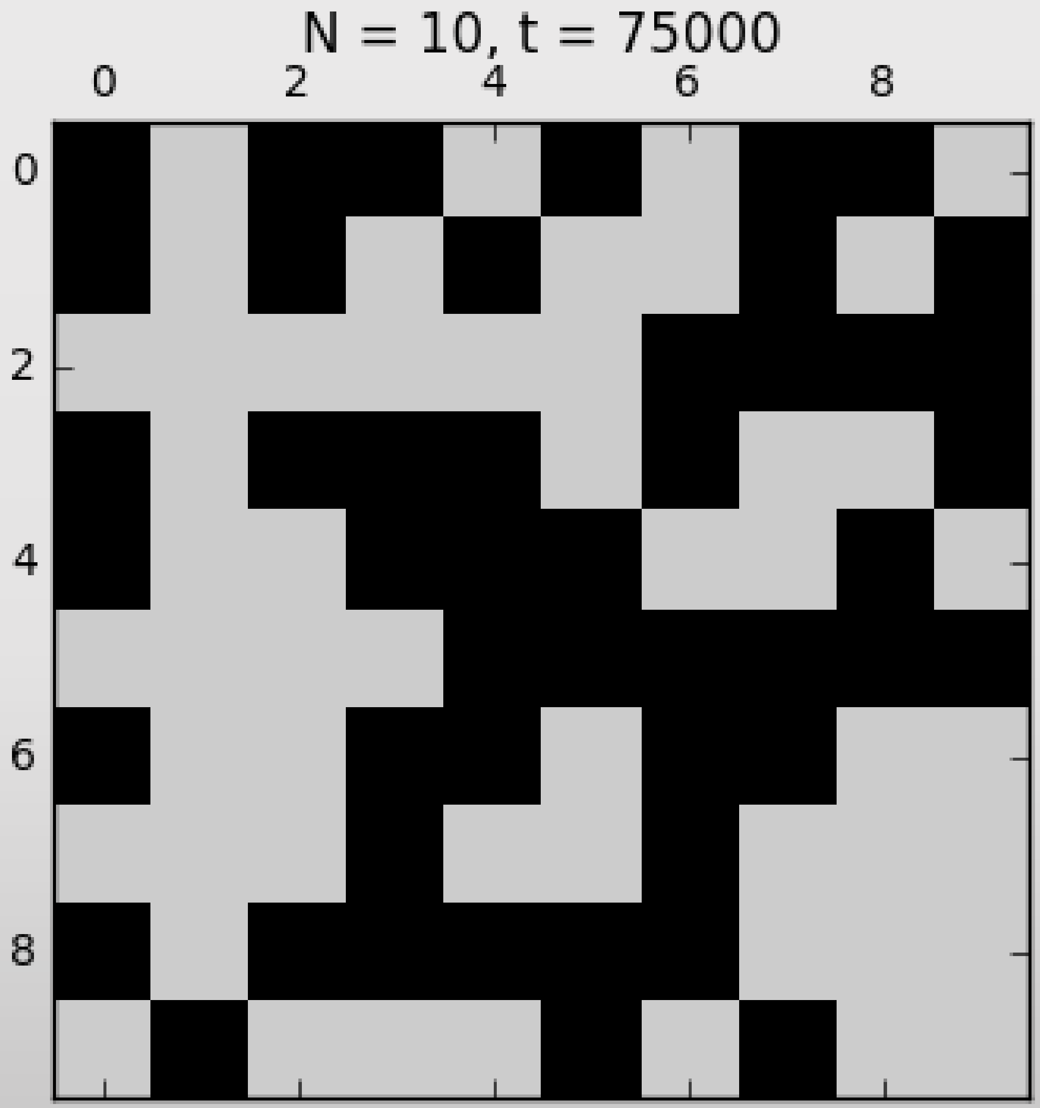
Sample 2D Spin Glass

$$kT = 0.5$$



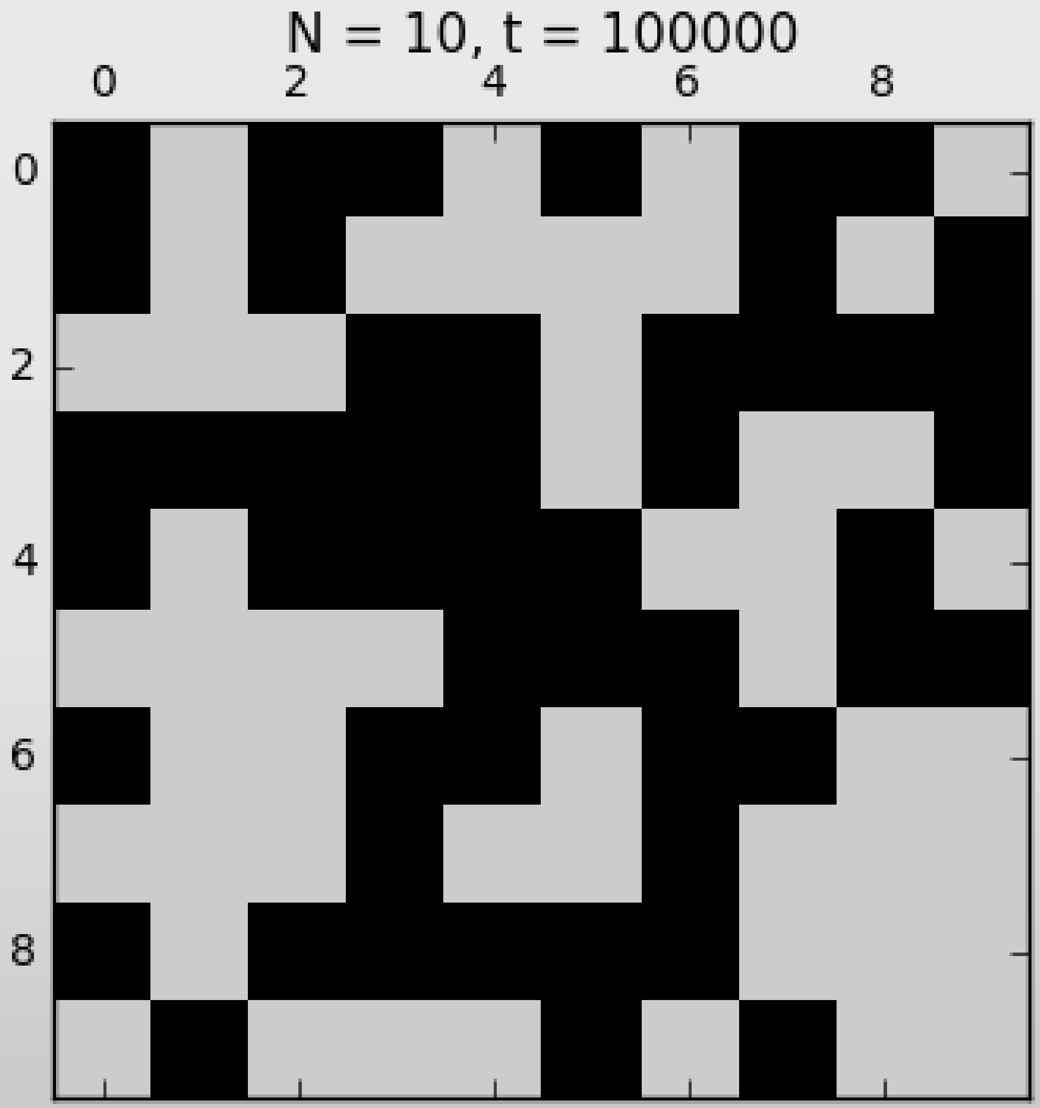
Sample 2D Spin Glass

$$kT = 0.5$$



Sample 2D Spin Glass

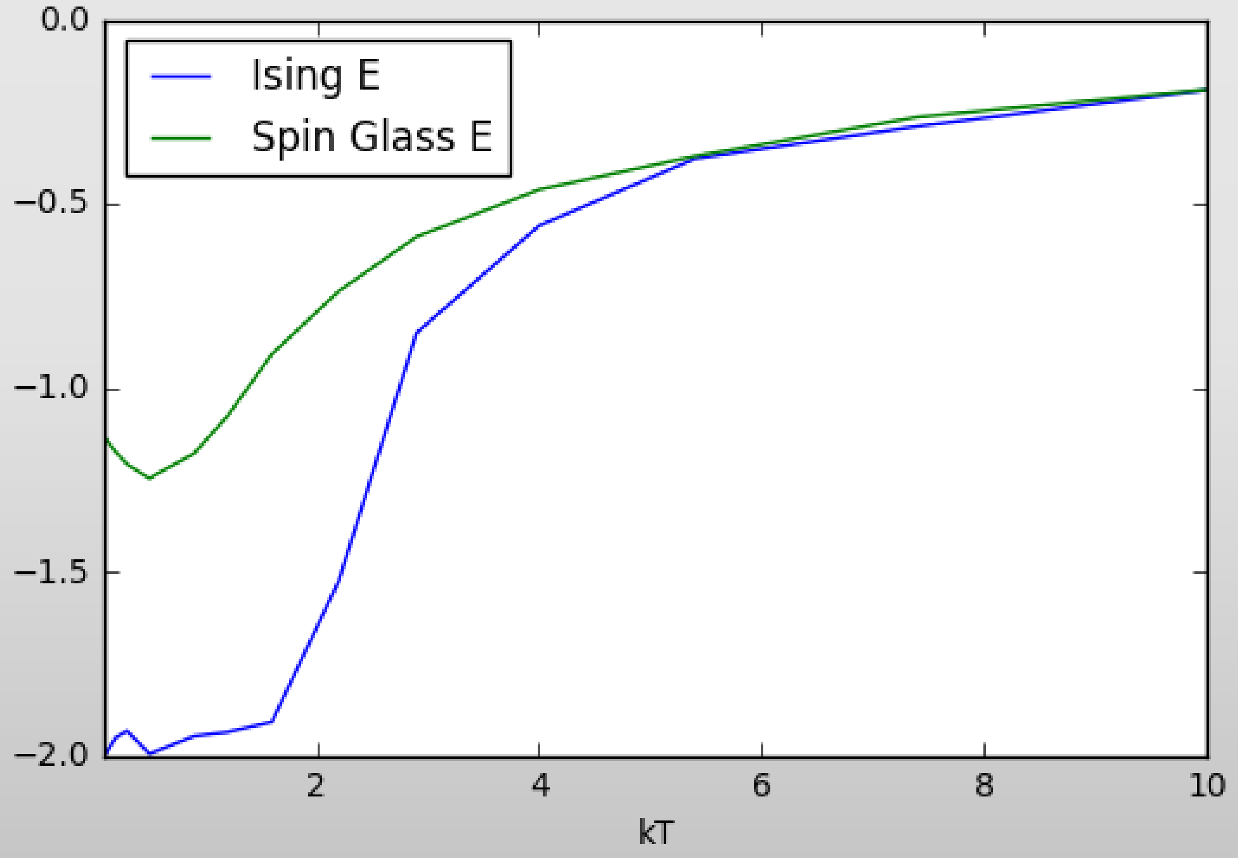
$$kT = 0.5$$



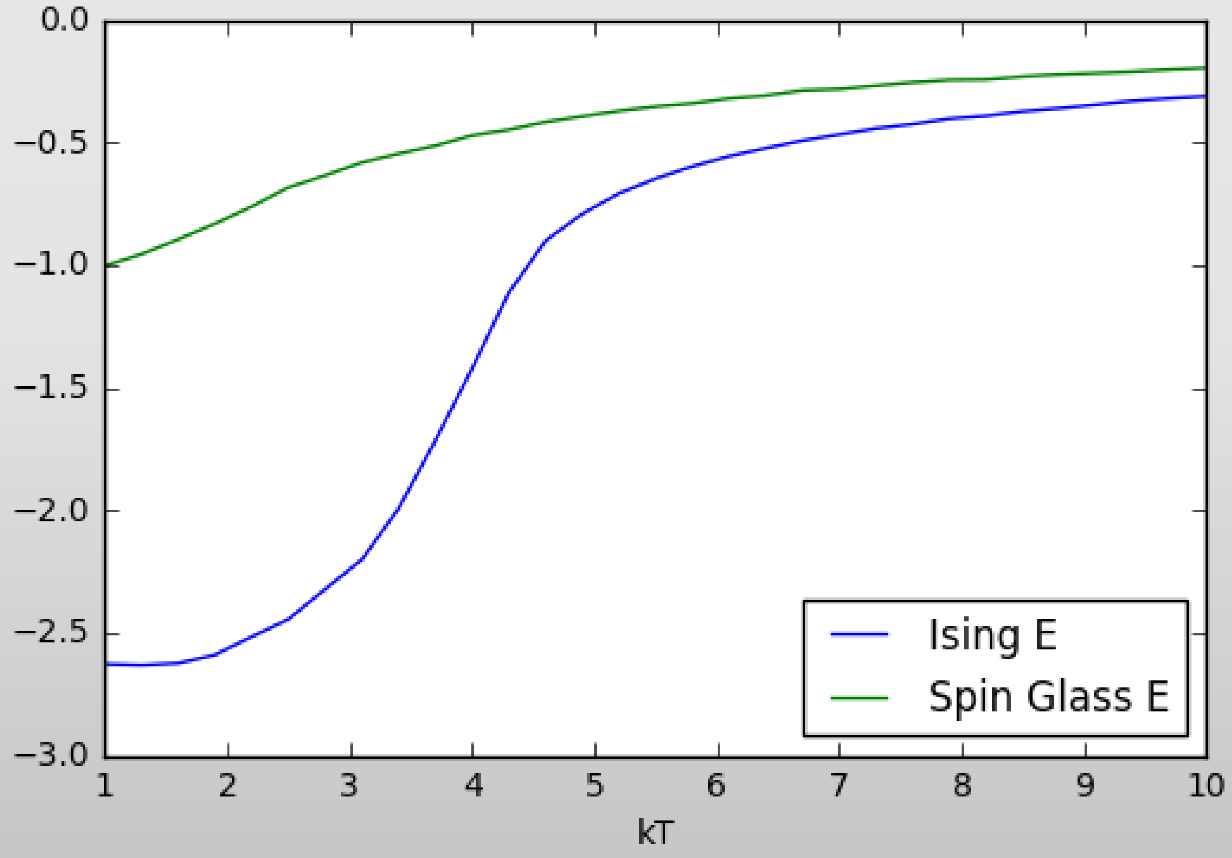
Spin Glasses are frustrated!

- Frustrated system → finding the lowest energy configuration is difficult. Hence, “glassy.”
- Use Monte Carlo methods to sample
  - Simulations at low T get stuck in local minima
  - Simulations at high T fail to explore deeper parts of the energy landscape

High T vs. Low T comparison, 2D



High T vs. Low T comparison, 3D



Parallel Tempering

- Run M simulations at once, each at different kT
- After a fixed number of spin flips, swap systems at adjacent temperatures with probability $\min(1, \exp(\Delta\beta\Delta E))$.
- Systems will explore a wide range of temperature, sampling within local minima and across the landscape
- (Must continue to obey detailed balance!)

Simulation Setup

kT=1	1.3	1.6	2.1	2.6	3.4	4.3	…
Replica 1	Replica 1	Replica 1	Replica 1	Replica 1	Replica 1	Replica 1	…
Replica 2	Replica 2	Replica 2	Replica 2	Replica 2	Replica 2	Replica 2	…

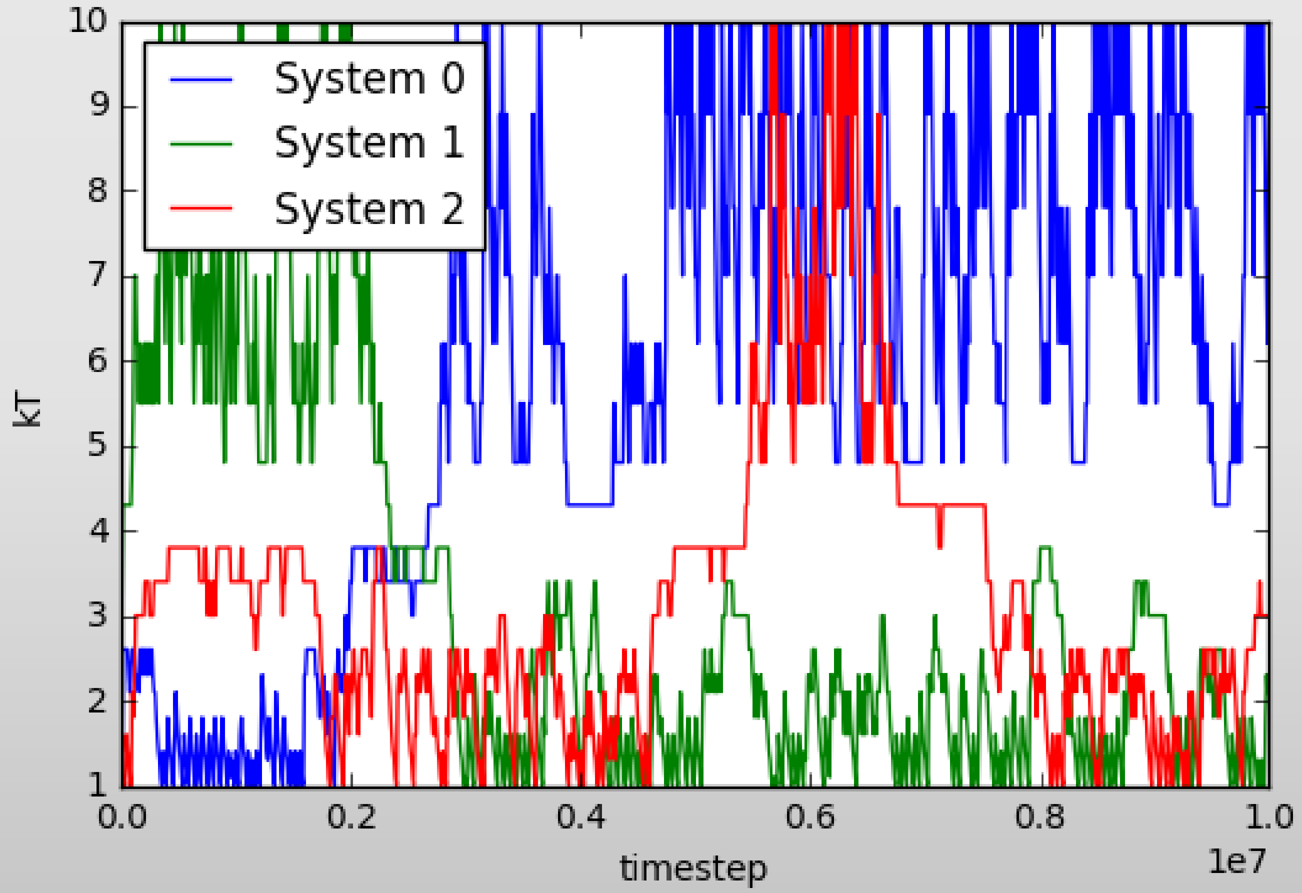
Control Parameters

- Range of temperatures
- Sweeps per global move
- Replicas at each kT

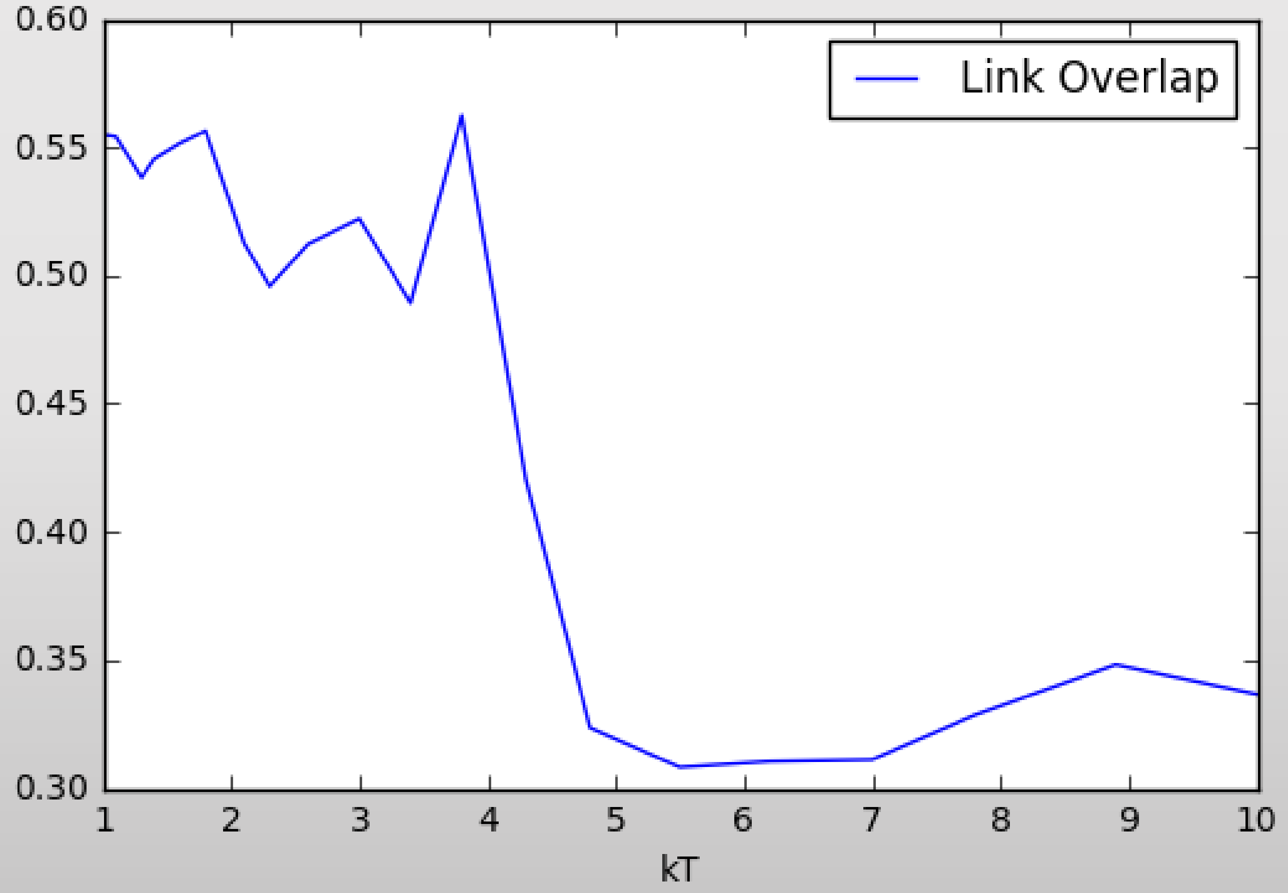
Output Parameters

- Average acceptance rate $A = \min(1, \exp(\Delta\beta\Delta E))$
  - “the acceptance rate for the trials depends on the likelihood that the system sampling the higher temperature happens to be in a region of phase space that is important at the lower temperature”
- Round trip time τ

3D Ising System Crossovers



3D Ising q_l, Link Overlap



$$q_l = \sum_{<i,j>} S_i^1 S_j^1 S_i^2 S_j^2$$

$$\langle q_l \rangle = 1 - \frac{2T|E|}{zJ^2}$$

Challenges & Optimization

- Max efficiency around 23% exchange?
  - (Disputes in lit. about best method)
- Minimize round-trip time τ
- Critical slowdown near phase transition
  - Increase temperatures near critical region

Katzgraber 2001, Bittner 2008

Applications of Parallel Tempering

- Polymers
- Biomolecules
- Quantum systems
- Cases where dynamics are *not* of interest, but energy minima are of interest

References

- [1] H. G. Katzgraber, M. Palassini, and A. P. Young, Phys. Rev. B **63**, 1 (2001).
- [2] D. J. Earl and M. W. Deem, Phys. Chem. Chem. Phys. **7**, 3910 (2005).
- [3] E. Bittner, A. Nußbaumer, and W. Janke, Phys. Rev. Lett. **101**, 1 (2008).

Q&A