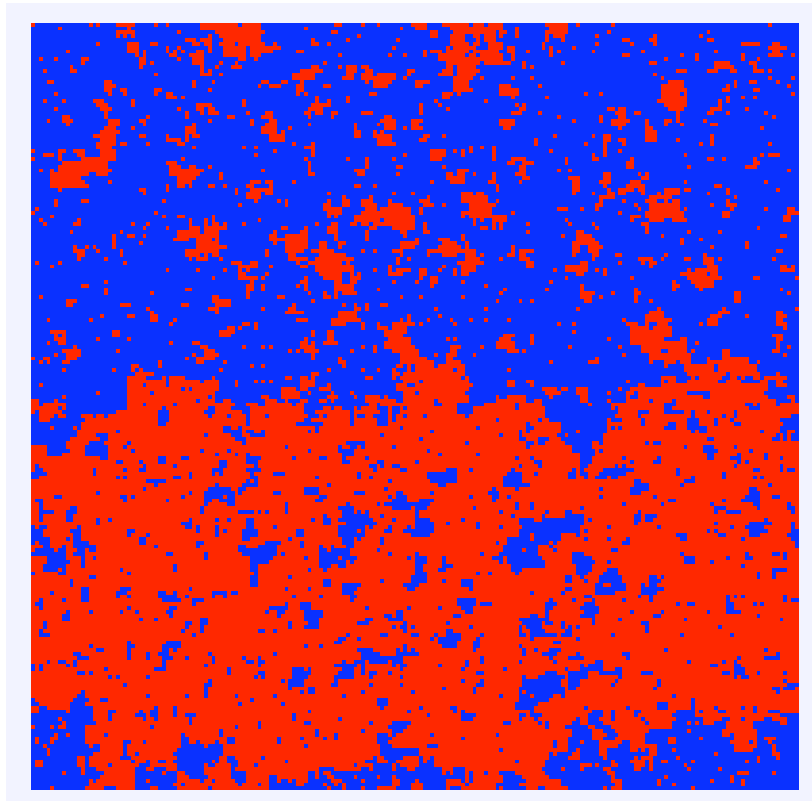
Simulating Glauber dynamics for the Ising model



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Why is it that many materials exhibit “spontaneous magnetization”?

- At low temperatures, they are magnetic.
- At high temperatures, they are not.

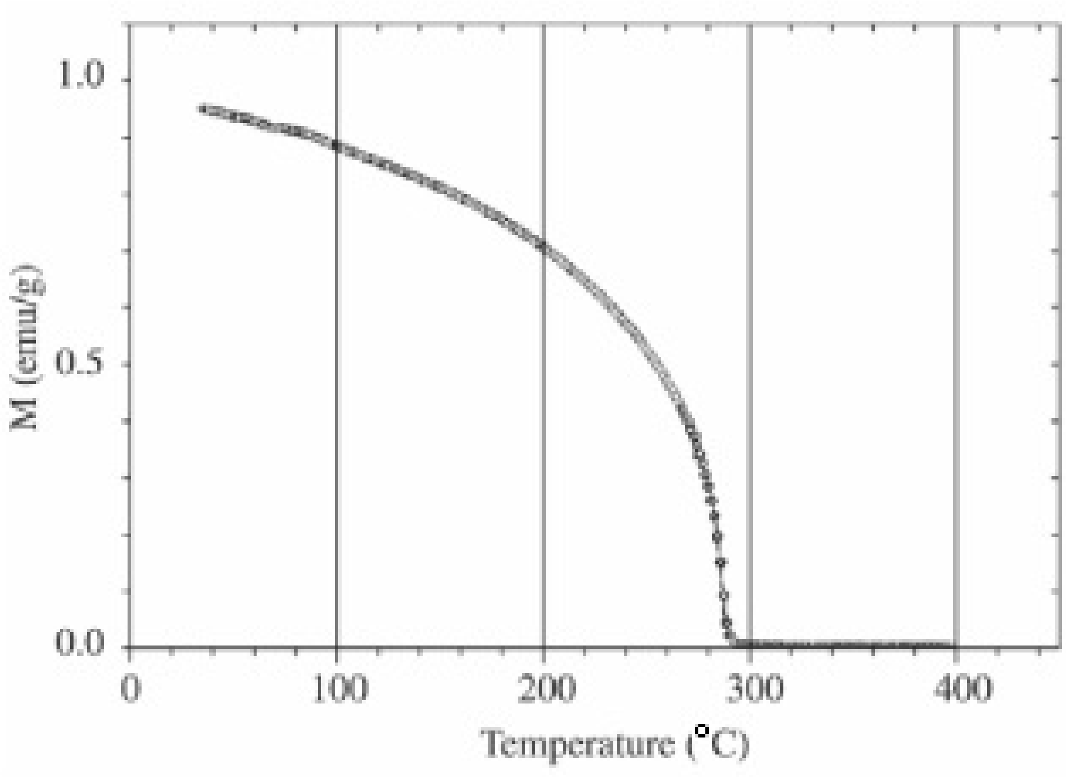


Figure 8. Magnetization-temperature curve of the powder calcined at 1450 °C when subsequently subjected to a 240 Oe magnetic field.

Electron “spins” and magnetization

- W. Lenz (1920) proposed a model of ferromagnetism. That each electron possesses a “spin”. Parallel spins attract. Antiparallel spins repel. At sufficiently low temperatures, the spins should align.

- Ernst Ising (1924), in his doctoral thesis advised by Lenz, formalized these ideas and examined a 1-D chain of such spins.

$$s_i \in \{-1, +1\}$$

$$\boxed{E_i \propto -s_i s_j}$$

the “exchange energy”

The "Ising" model

- Consider a 2-D lattice.
- At each site is a spin, $s_i \in \{-1, +1\}$.
- Spins interact only with nearest neighbors.
- There can be an external field h.
- Thus the energy for each spin, E_i:

$$E_i = -\sum_{\{s_j\}} J_{ij} s_i s_j - h s_i$$

Total energy, the "Hamiltonian"

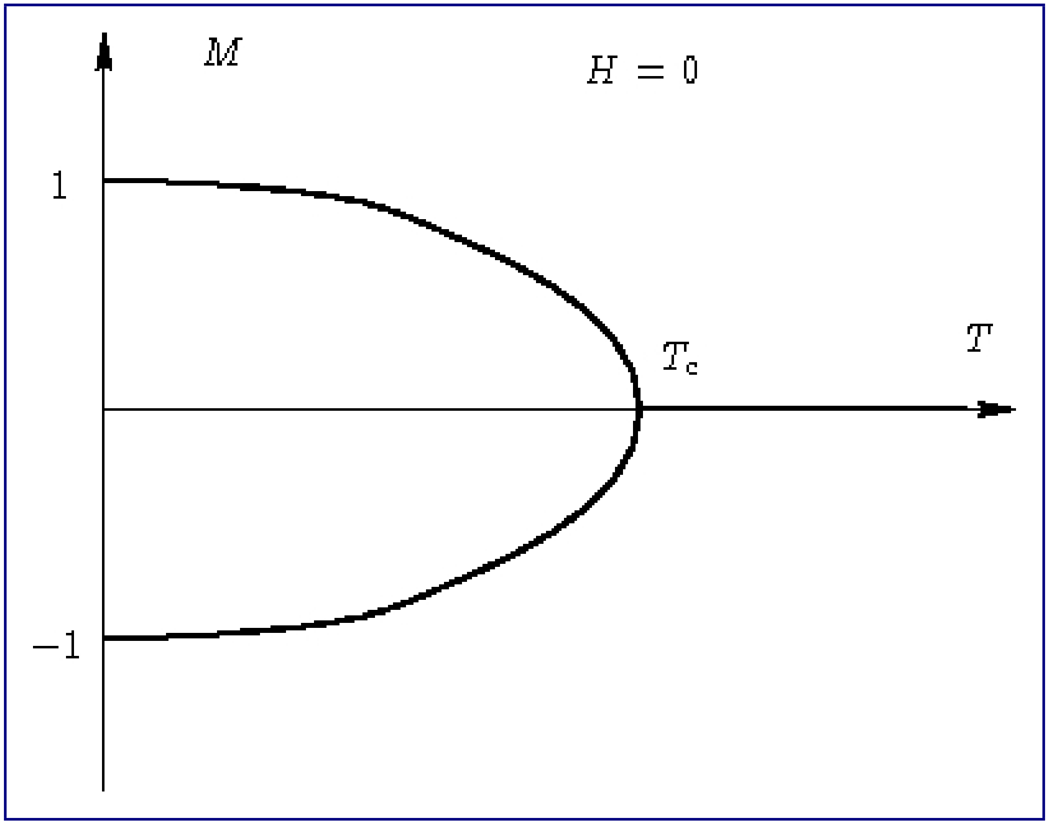
$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} s_i s_j - \sum_i h s_i$$

- The first sum is over all nearest neighbor pairs.
- J_{ij} is the coupling between spins. We take $J_{ij} = J = 1$.
- Set external field $h = 0$ (if not, hysteresis).
  - Hysteresis enables magnetic storage of data.
  - Avalanche phenomena in domain flipping.
  - Studied via Random Field Ising Models (RFIM).

Magnetization, M

$$M = \frac{1}{N}\sum_i s_i$$

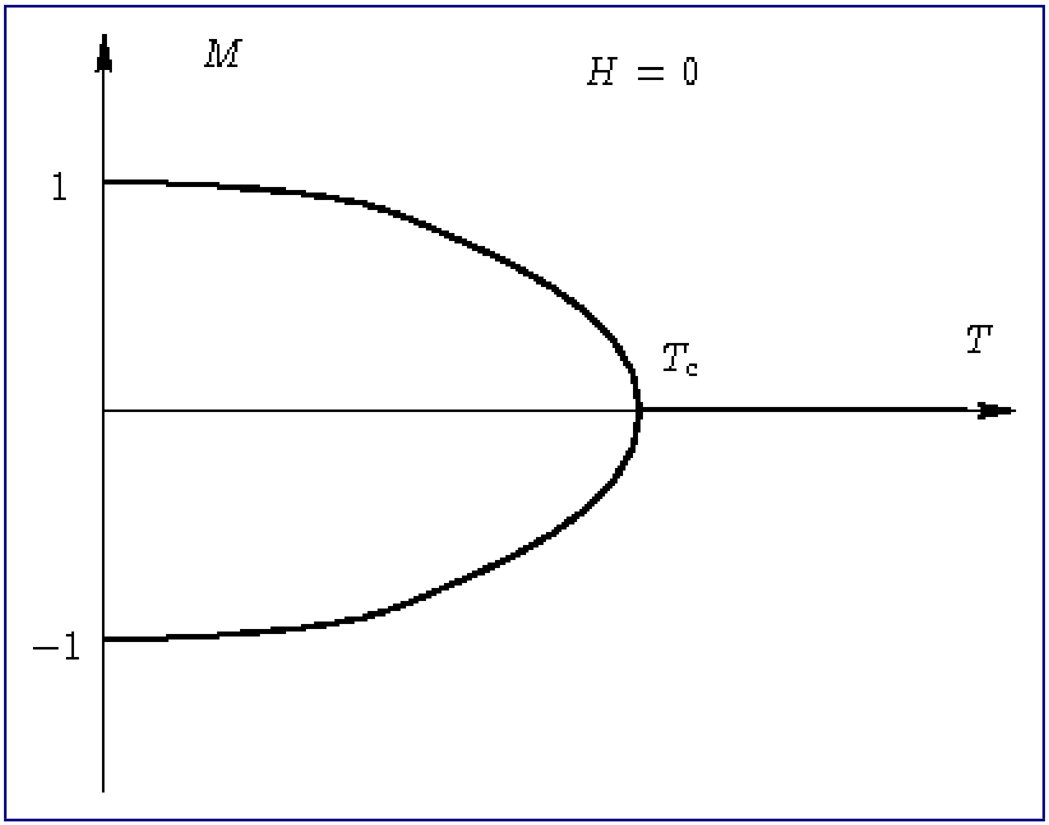
- All spins "up" $\rightarrow M = 1.$
- All spins "down" $\rightarrow M = -1.$



Phase transition in M as function of T

- Peierls (1936), gave a non-rigorous proof that spontaneous magnetization must exist for the 2-D Ising model.

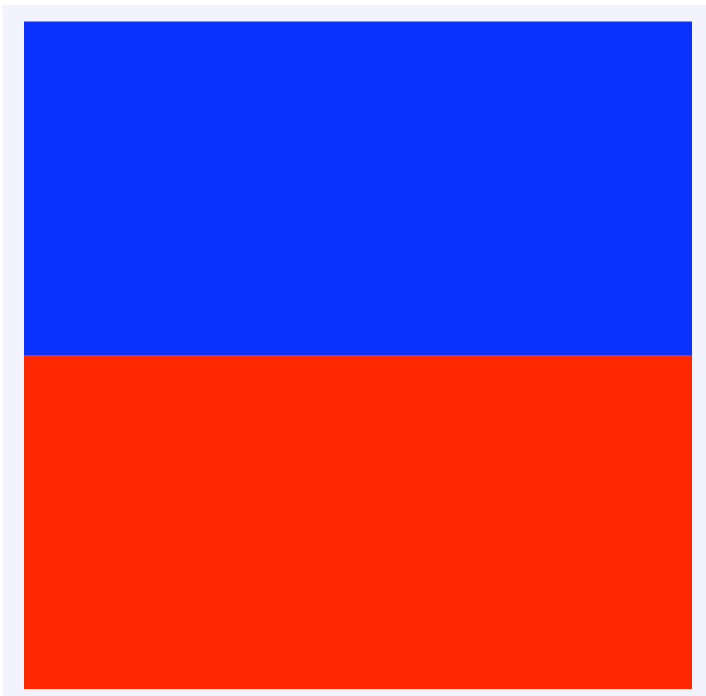
- Onsager (1944), gave a complete analytic solution.

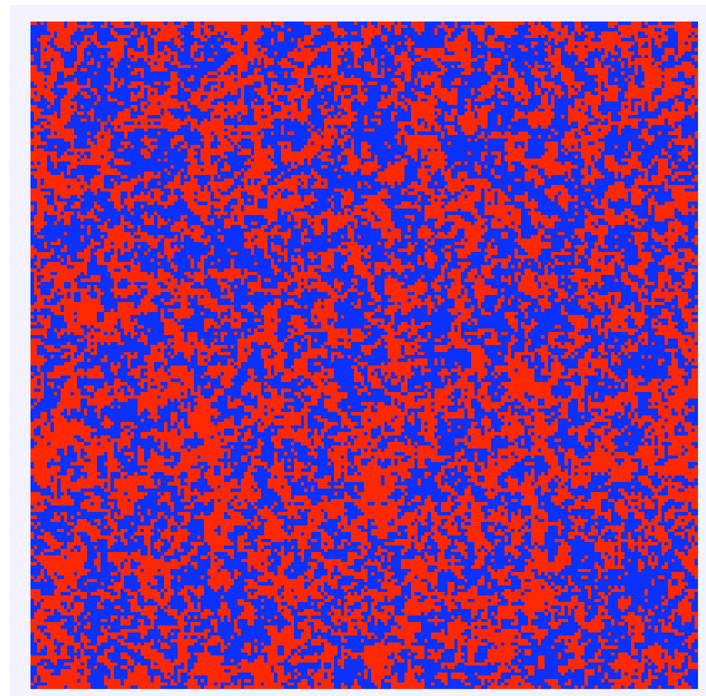


Phase transitions and universality — more on this later!

How to simulate the Ising model?

- Starting from any initial condition, we know the equilibrium value of the magnetization. It is a function only of Temperature. How do we get to equilibrium?





$\longrightarrow$

Equilibrium

- In equilibrium, Boltzmann probability:

$$p(E_i) = e^{(-E_i/kT)}/z$$

- E_i is energy of state i.
- k is Boltzmann's constant.
- T is temperature.
- $z = \sum_i e^{-E_i/kT}$ is the partition (i.e., generating) function.

Spin-flip algorithms
"Monte Carlo"

- Use a stream of random numbers to drive a stochastic process, in this case the generation of a succession of many states of the spin model.

- For an $L \times L$ lattice, there are $2^{L\times L}$ states. (e.g., If $L = 10$, there are 2^{100} possible states).

- Want to sample the phase space so that each state occurs with the same probability as its equilibrium probability.

- Metropolis (1953) detailed balance ensures convergence to equilibrium.

$$P(S_i)P(S_i \to S_j) = P(S_j)P(S_j \to S_i)$$

Detailed balance

$$P(S_i)P(S_i \rightarrow S_j) = P(S_j)P(S_j \rightarrow S_i)$$

in other words:

$$\frac{P(S_i \rightarrow S_j)}{P(S_j \rightarrow S_i)} = \frac{P(S_j)}{P(S_i)} = e^{-(E_j - E_i)/kT}$$

(Where the last equality follows from the Boltzmann probability).

Glauber dynamics

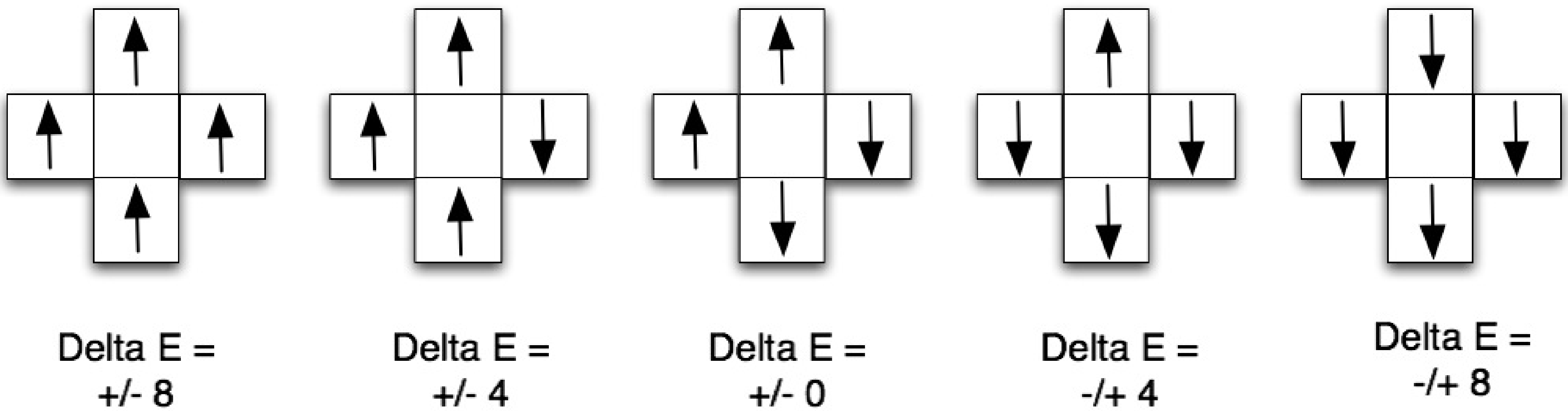
- $P(S_i \rightarrow S_j) = e^{-E_j/kT}/(e^{-E_j/kT} + e^{-E_i/kT})$

$$= 1/(1 + e^{\Delta E_{ji}/kT})$$

- Choose a spin a random.
- Calculate the energy difference resulting if that spin were flipped: ΔE.
- Transition probability: $P(\text{flip}) = 1/(1 + \mathrm{e}^{\Delta \mathrm{E}/\mathrm{kT}})$.
- Generate a random number, X. If $X < P(\text{flip})$ accept.
- Parameterize time such that one unit of time is N spin-flip attempts.

Implementing the Glauber dynamics

- Only a finite number (5) of possible energy changes.
- Can pre-compute the probabilities, $1/(1+e^{\Delta E/kT})$.



Simulations

- High temperature (initial condition irrelevant)

- Low temperature (initial condition “quenched”)

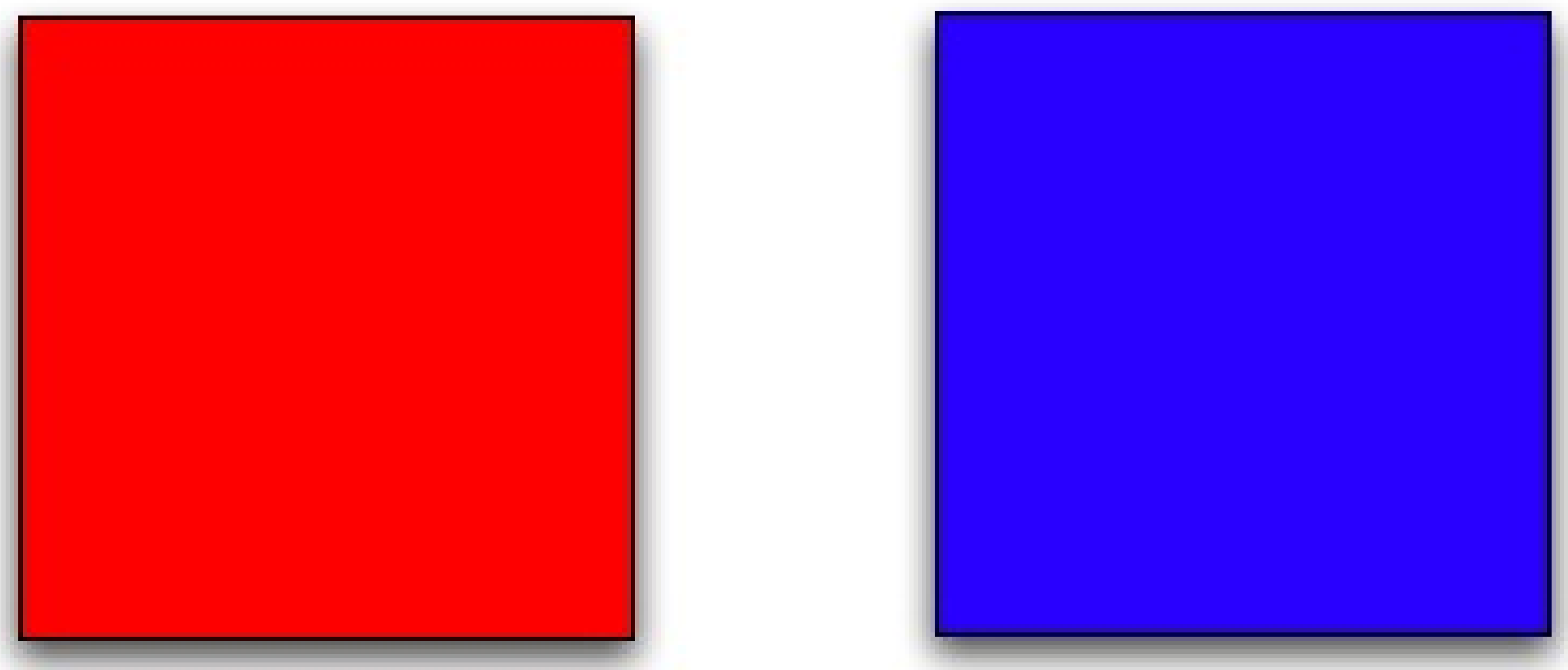
- Critical temperature (???)

Issues

- Critical slowing down (correlation length diverges), and so does the relaxation time....

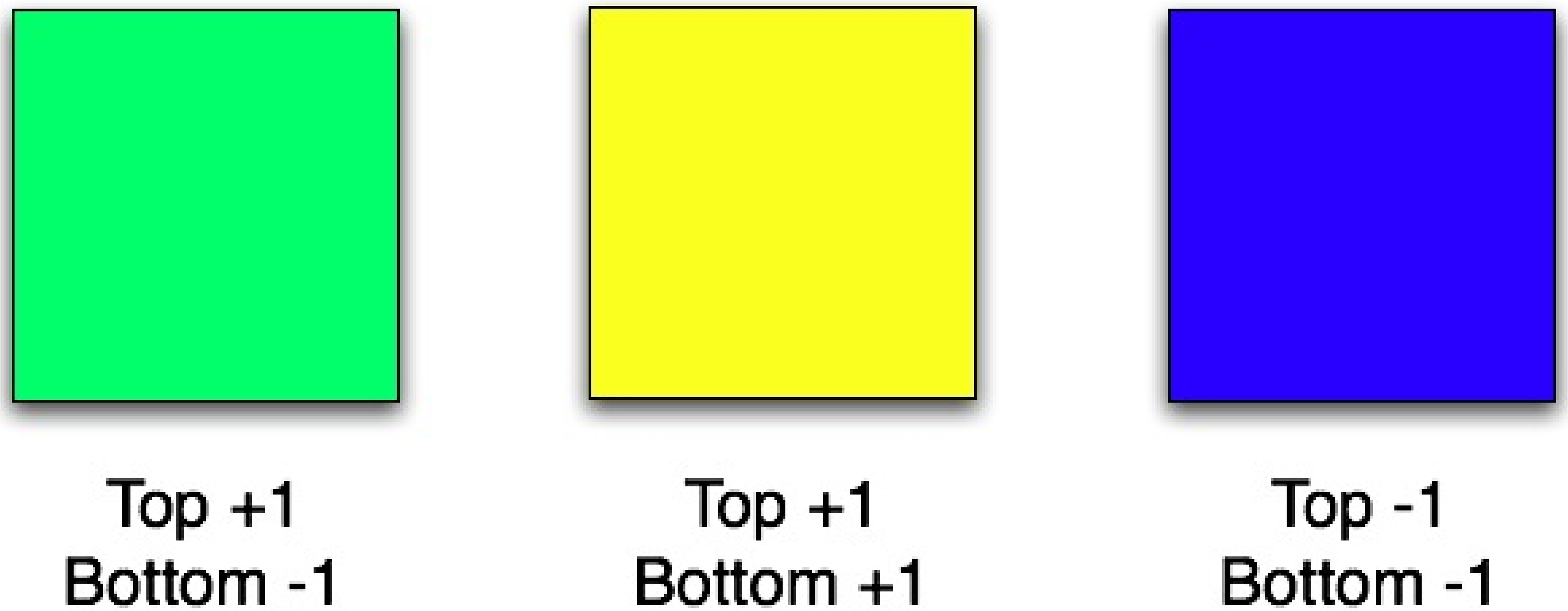
- The critical point is the most interesting, yet the hardest to access and pin down!

A coupled dynamics



- “Top” copy all spin up, +1.
- “Bottom” copy all spin down, -1.

Greedy coupled dynamics



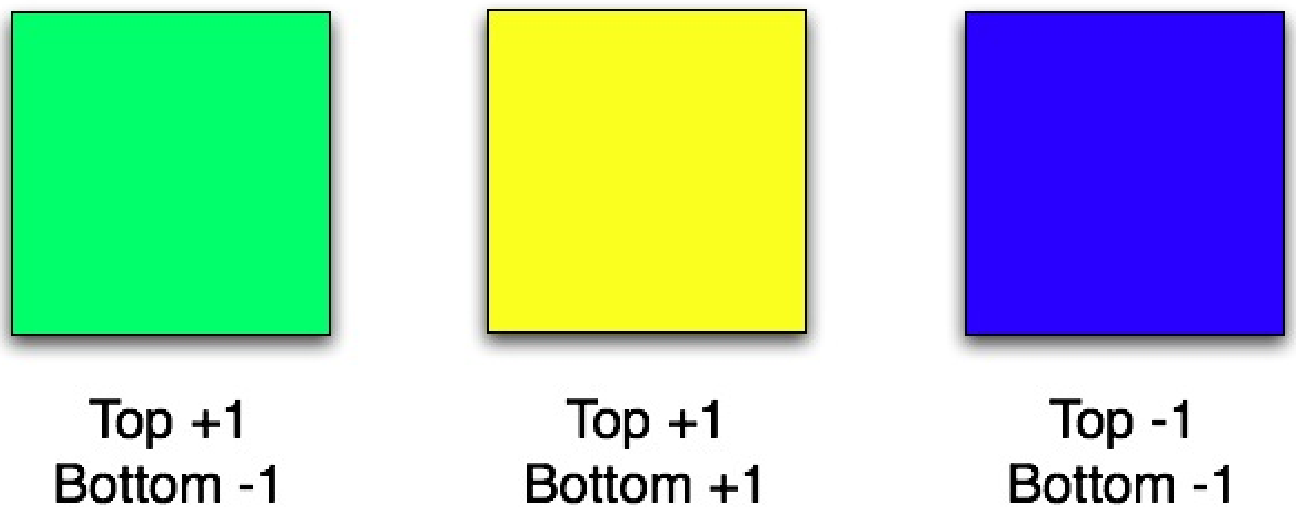
- Pick a lattice site, v, at random.
- Calculate probability for spin s_v to be +1 in the top, p_{top}.
- Calculate probability for spin s_v to be +1 in the bottom, p_{bot}.

Probabilities (as usual)

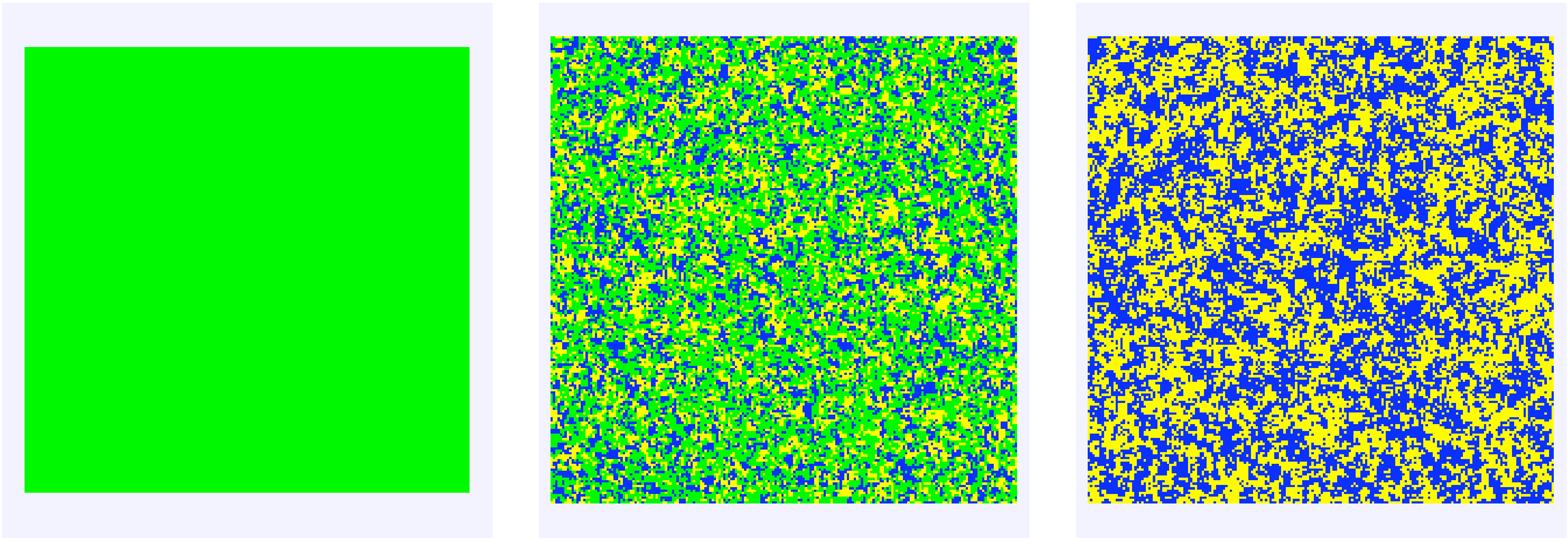
$$p(+) = \frac{e^{-E(+)\beta}}{e^{-E(+)\beta} + e^{-E(-)\beta}}$$

Dynamics

- Generate a random number, X.
- set s_v to be blue if: $X < p_{bot}$.
- set s_v to be green if: $p_{bot} < X < p_{top}$.
- set s_v to be yellow if: $X > p_{top}$.



The coupled system



Growth of coupling with time.

Online Resources

Ising model simulation:

- http://stp.clarku.edu/simulations/ising2d/
- http://bartok.ucsc.edu/peter/java/ising/keep/ising.html

Cluster-flip dynamics:

- http://www.hermetic.ch/compsci/thesis/chap1.htm