A gentle introduction to the Potts Model

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With a little (*a lot of!*) help from my friends….

- Laura Beaudin (SMC 2006)
- Patti Bodkin (SMC 2004)
- Mary Cox (UVM grad)
- Whitney Sherman (SMC 2004)

VGN INBRE NIH

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The Ising Model

1925—(Lenz)

Consider a sheet of metal:

It has the property that at low temperatures it is magnetized, but as the temperature increases, the magnetism “melts away”.

We would like to model this behavior. We make some simplifying assumptions to do so.

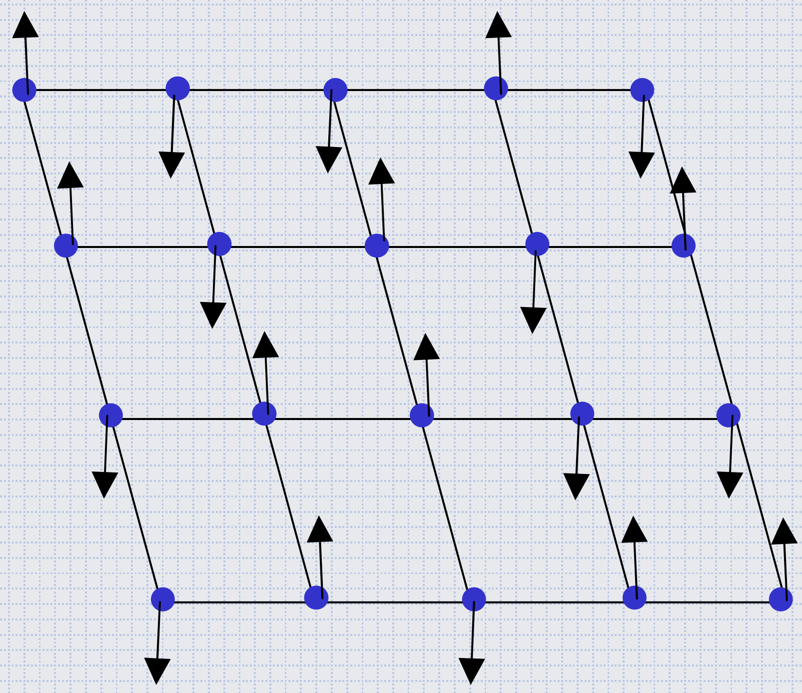
– The individual atoms have a “spin”, i.e., they act like little bar magnets, and can either point up (a spin of +1), or down (a spin of –1).

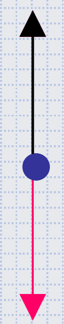
– Neighboring atoms with different spins have an interaction energy, which we will assume is constant.

– The atoms are arranged in a regular lattice.

One possible state of the lattice

A choice of ‘spin’ at each lattice point.





$q = 2$

Ising Model has a choice of two possible spins at each point

The Kronecker delta function and the Hamiltonian of a state

Kronecker delta-function is defined as:

$$\delta_{a,b} = \begin{cases} 0 & \text{for } a \neq b \\ 1 & \text{for } a = b \end{cases}$$

The *Hamiltonian* of a system is the sum of the energies on edges with endpoints having the same spins.

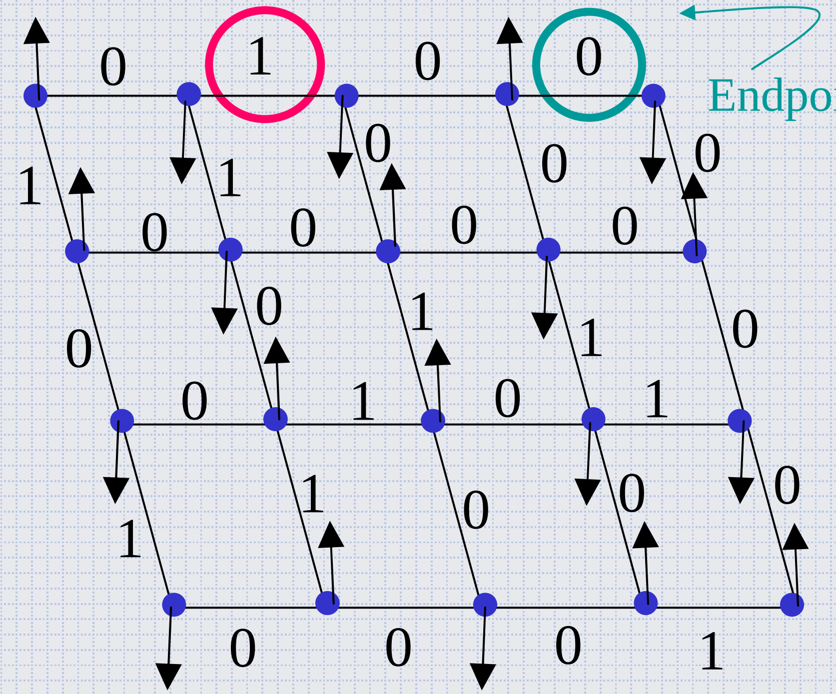
$$H = \sum_{edges} -J \ \delta(a,b)$$

where a and b are the endpoints of the edge, and J is the energy of the edge.

The energy (Hamiltonian) of the state

Endpoints have the same spins, so δ is 1.

Endpoints have different spins, so δ is 0.



$$H(w) = \sum_{edges} -J\delta_{s_i,s_j}$$

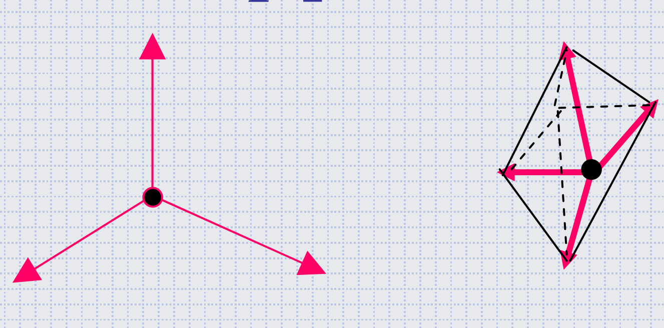
$H(w)$ of this system is -10J

A state w with the value of δ marked on each edge.

The Potts Model

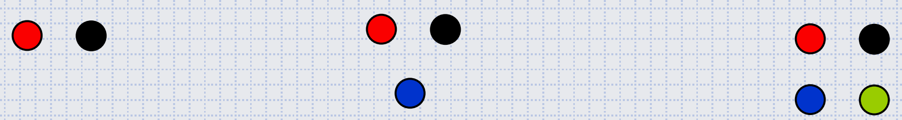
1952—(Domb)

Now let there be q possible states….

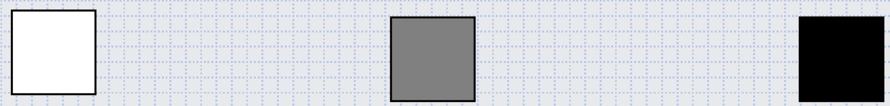


$q = 2$ $q = 3$ $q = 4$

Orthogonal vectors, with δ replaced by dot product



Colorings of the points with q colors



Healthy Sick Necrotic

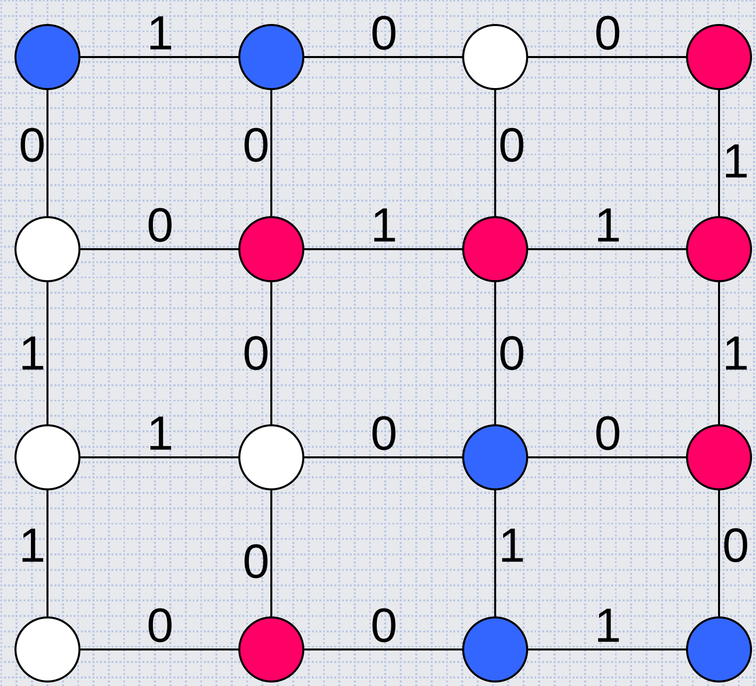
States pertinent to the application

More states--Same Hamiltonian

- The **Hamiltonian** still measures the overall energy of the a state of a system.

$$H(w) = \sum_{edges} -J\delta_{s_i, s_j}$$

The Hamiltonian of a state of a 4X4 lattice with 3 choices of spins (colors) for each element.



$$H = -10J$$

Probability of a state

The probability of a particular state S occurring depends on the *temperature, T*

(or other measure of activity level in the application)

$$P(S) = \frac{\exp(-\beta H(S))}{\sum_{\text{all states } \mathbf{S}} \exp(-\beta H(\mathbf{S}))}$$

$\beta = \frac{1}{kT}$ where $k = 1.38 \times 10^{-23}$ joules/Kelvin and T is the temperature of the system.

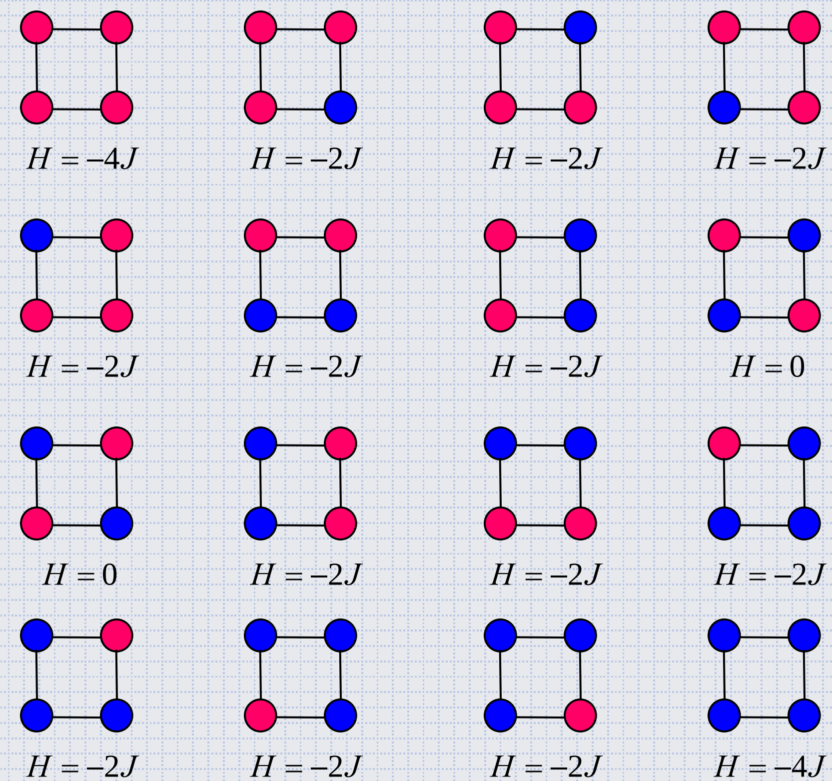
The numerator is easy. The denominator, called the *Potts Model Partition Function,* is the interesting (hard) piece.

Example

$$P(S) = \frac{\exp(-\beta H(S))}{\sum_{\text{all states } \mathbf{S}} \exp(-\beta H(\mathbf{S}))}$$

$$P(\text{all red}) = \frac{\exp(4\beta J)}{12\exp(2\beta J) + 2\exp(4\beta J) + 2}$$

The Potts model partition function of a square lattice with two possible spins on each element.



$$\boxed{12\exp(2J\beta) + 2\exp(4J\beta) + 2}$$

Probability of a state occurring depends on the temperature

P(all red, T=0.01) = .50 or 50%

P(all red, T=2.29) = 0.19 or 19%

P(all red, T = 100, 000) = 0.0625 = 1/16

(Setting J = k for convenience)

Effect of Temperature

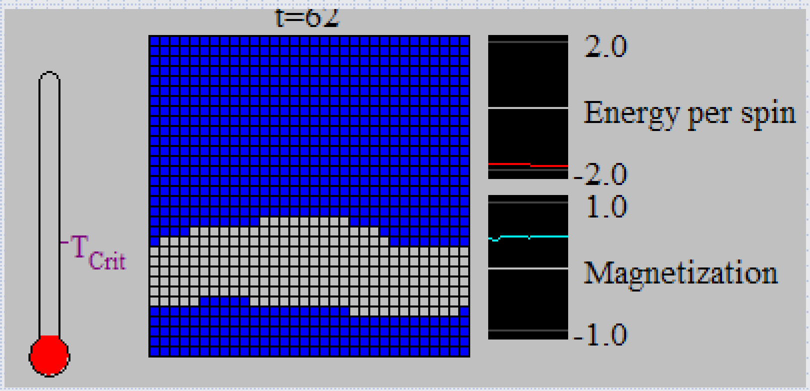
- Consider two different states **A** and **B**, with ***H*(*A*) < *H*(*B*)**. The relative probability that the system is in the two states is:

$$\frac{P(A)}{P(B)} = \frac{e^{-\beta H(A)}}{\sum_{\text{all states } \mathbf{S}} e^{-\beta H(\mathbf{S})}} \Bigg/ \frac{e^{-\beta H(B)}}{\sum_{\text{all states } \mathbf{S}} e^{-\beta H(\mathbf{S})}}$$

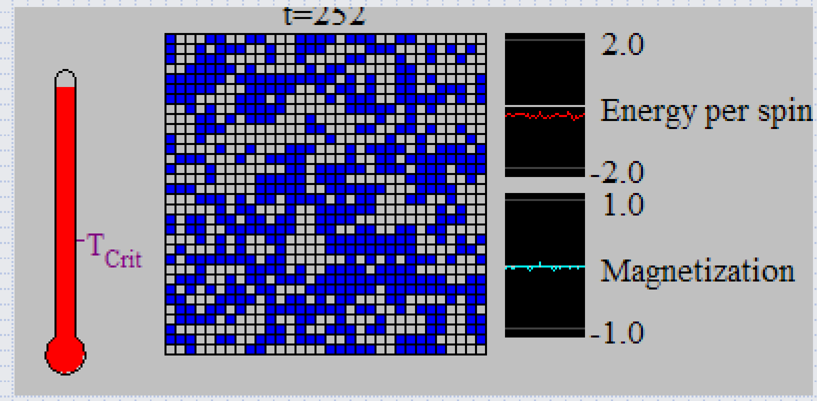
$$= \frac{e^{-\beta H(A)}}{e^{-\beta H(B)}} = e^{-\frac{D}{kT}} = e^{\frac{|D|}{kT}}, \text{ where } D = H(A) - H(B) < 0.$$

- At high temperatures (i.e., for ***kT*** much larger than the energy difference |**D**|), the system becomes equally likely to be in either of the states **A** or **B** - that is, randomness and entropy "win". On the other hand, if the energy difference is much larger than ***kT***, the system is far more likely to be in the lower energy state.

Ising Model at different temperatures



Cold Temperature



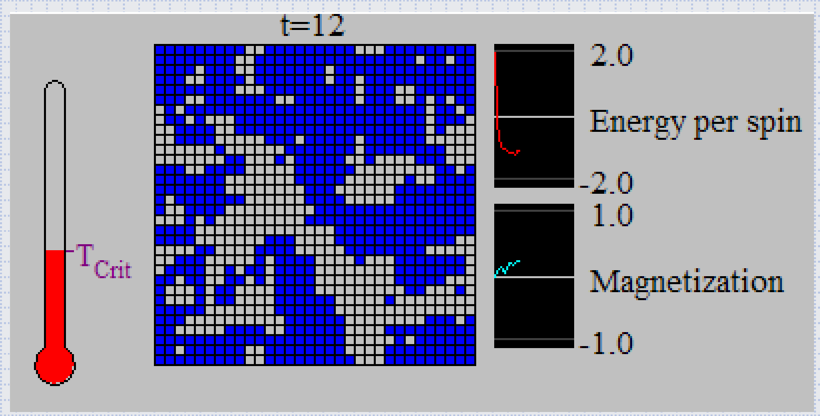
Hot Temperature

Here H is

$$\sum s_i s_j$$

and energy is

$$\frac{H}{\#\ \text{of squares}}$$



Critical Temperature

Images from http://bartok.ucsc.edu/peter/java/ising/keep/ising.html
http://bartok.ucsc.edu/peter/java/ising/isingAppletLarge.html

Applications of the Potts Model

(about 1,000,000 Google hits…)

- **Liquid-gas transitions**
- **Foam behaviors**
- **Protein Folds**
- **Biological Membranes**
- **Social Behavior**
- **Separation in binary alloys**
- **Spin glasses**
- **Neural Networks**
- **Flocking birds**
- **Beating heart cells**

Complex Systems with nearest neighbor interactions….

A personal favorite…

Y. Jiang, J. Glazier, *Foam Drainage: Extended Large-Q Potts Model Simulation*

We study foam drainage using the large-Q Potts model... profiles of draining beer foams, whipped cream, and egg white ...

3D model: http://www.lactamme.polytechnique.fr/Mosaic/images/ISIN.41.16.D/display.html

Physical Application

- "Foams are of practical importance in applications as diverse as brewing, lubrication, oil recovery, and fire fighting".

$$H = \sum_{\{i,j\}} J(1-\delta_{\sigma_i \sigma_j}) + \lambda \sum_n (a_n - A_n)^2$$

- The energy function is modified by the **area** of a bubble.

Results:

Larger bubbles flow faster.

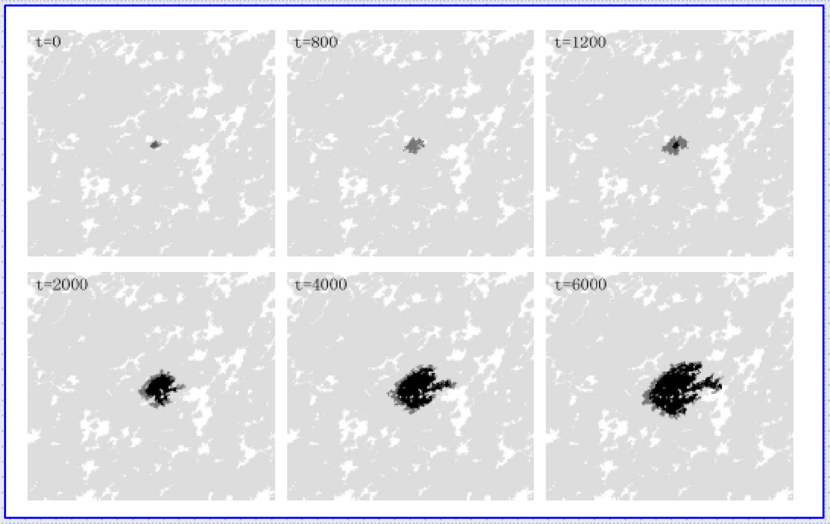
There is a **critical velocity** at which the foam starts to flow uncontrollably

Biological Application

- This model was developed to see if tumor growth is influenced by the amount and location of a **nutrient**.

$$H=\sum_{ij}\sum_{ij}J_{\tau(\sigma_{ij})\tau(\sigma_{i'j'})}\left\{1-\delta_{\sigma_{ij}\sigma_{i'j'}}\right\}+\sum_{\sigma}\lambda(v_{\sigma}-V_{T})^{2}+Kp(i,j)$$

- Energy function is modified by the volume of a cell and the amount of nutrients.



Results:

Tumors grow **exponentially** in the beginning.

The tumor migrated **toward** the nutrient.

Sociological Application

- The Potts model may be used to "examine some of the individual incentives, and perceptions of difference, that can lead collectively to **segregation** …".
- (T. C. Schelling won the 2005 Nobel prize in economics for this work)

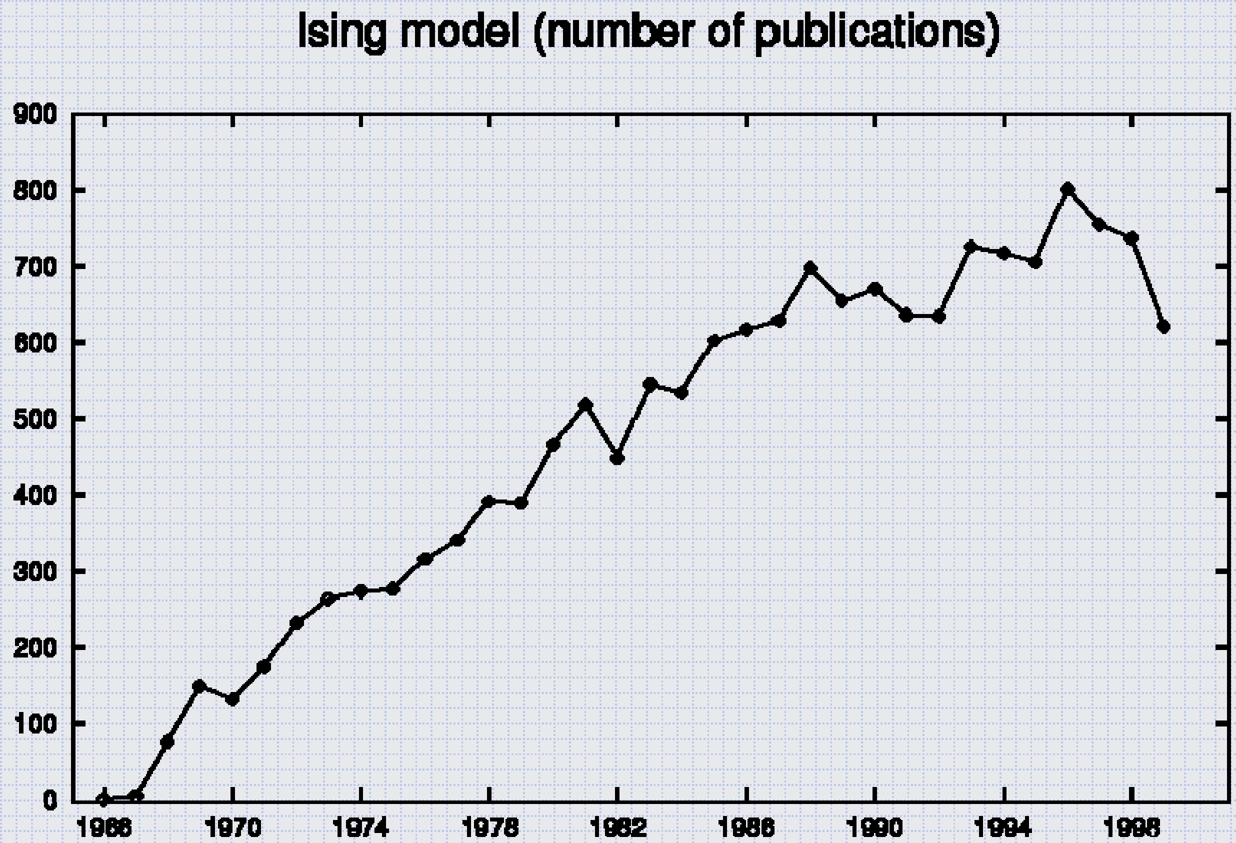
Variables:

Preferences of individuals

Size of the neighborhoods

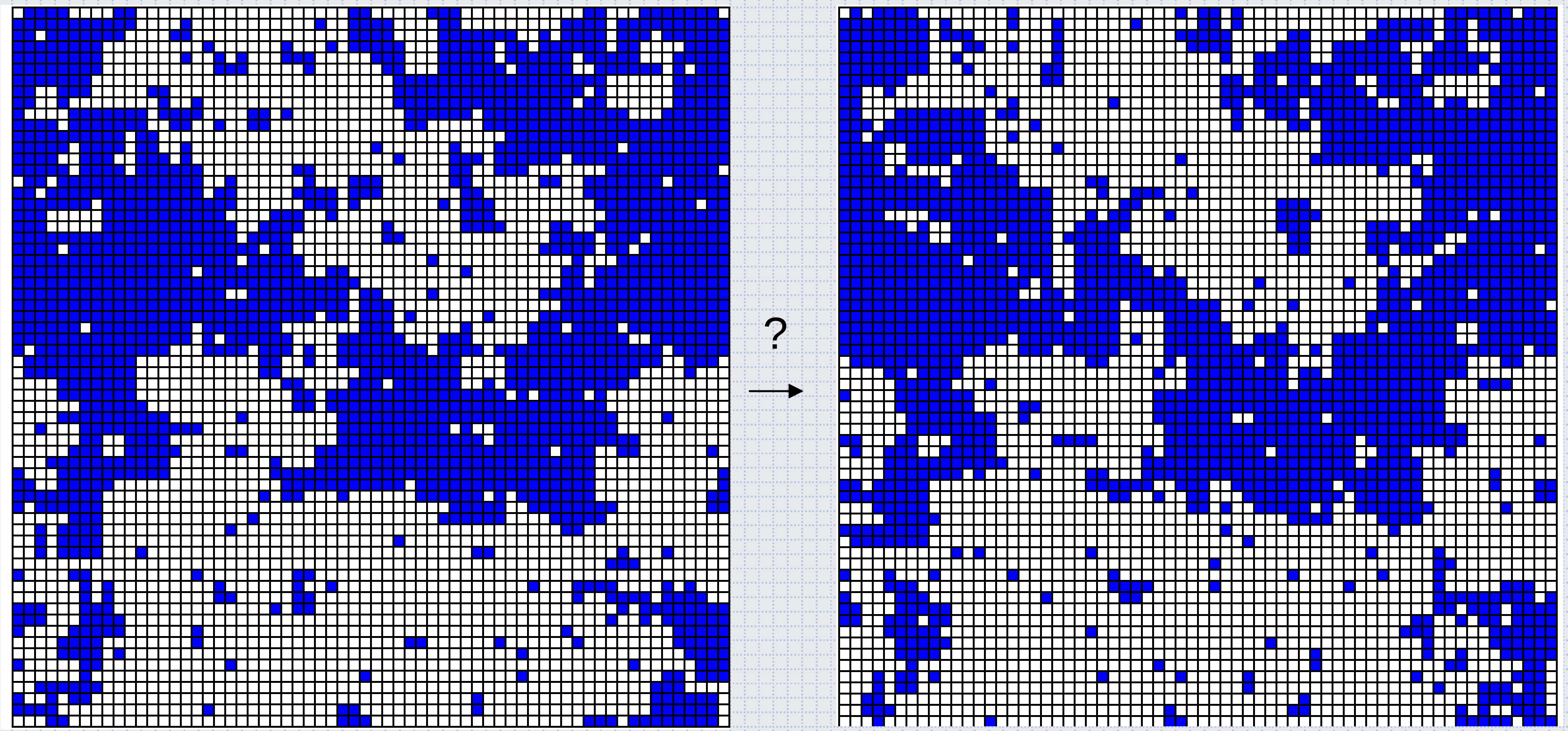
Number of individuals

Ernst Ising 1900-1998

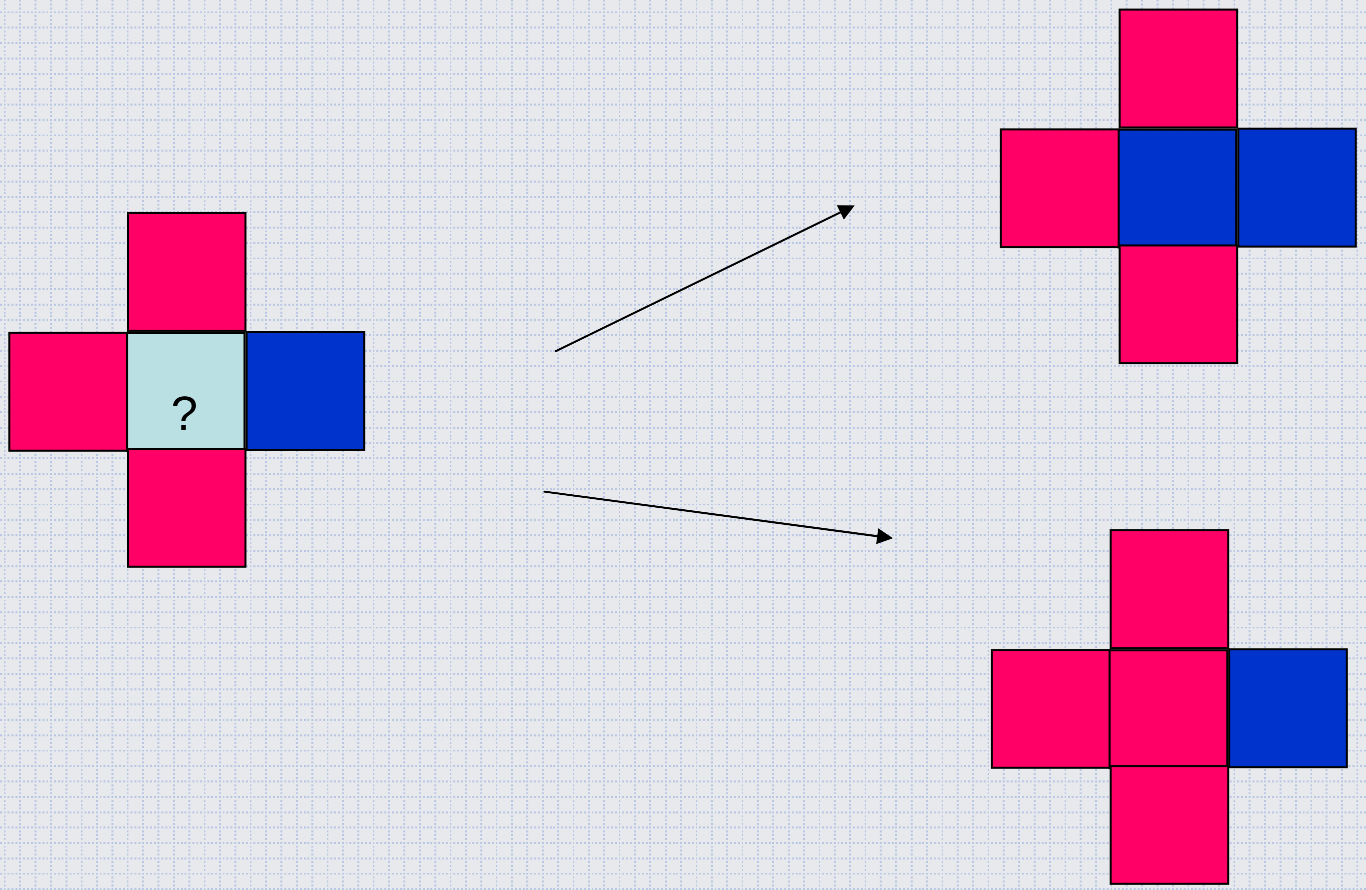


http://www.physik.tu-dresden.de/itp/members/kobe/isingconf.html

Monte Carlo Simulations



Monte Carlo Simulations



Thank you for attending!

- Questions?