

Simulations in Statistical Physics

Course for MSc physics students

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Ising-model

- ▶ Spins
 - ▶ Interact with external field h_i
 - ▶ Interact with neighbors with coeff. J_{ij}
- ▶ The Hamiltonian:

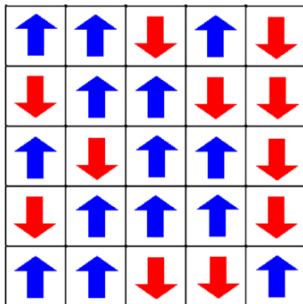
$$H(\sigma) = - \sum_{\langle i j \rangle} J_{ij} \sigma_i \sigma_j - \mu \sum_i h_i \sigma_i$$

- ▶ Order parameter magnetization

$$M = \sum_i \sigma_i$$

2D Ising-model

- ▶ 2 dimensions
- ▶ Homogeneous interaction: $J_{ij} = J$
- ▶ No external field (for the time being) $h = 0$



Importance sampling

- ▶ Given a Hamiltonian $H(\mathbf{q}, \mathbf{p})$
- ▶ We ask for the time average of a dynamics quantity at temperature T

$$\bar{A} = \int A(\mathbf{q}, \mathbf{p}) P^{eq}(\mathbf{q}, \mathbf{p}, T) d\mathbf{q} d\mathbf{p}$$

- ▶ In the canonical ensemble

$$P^{eq}(\mathbf{q}, \mathbf{p}, T) = \frac{1}{Z} e^{-\beta H(\mathbf{q}, \mathbf{p})}$$

- ▶ If A depends only on the energy (often the case):

$$\bar{A} = \int A(E) \omega(E) P^{eq}(E, T) dE$$

Importance sampling is needed!

Importance sampling

- ▶ $\omega(E)P^{eq}(E, T)$ has a very sharp peak (for large N)
- ▶ System spends most of its time *in equilibrium*
- ▶ Importance sampling:

Generate configurations with the equilibrium probability

- ▶ if configurations are chosen accordingly, the for K measurements:

$$\bar{A} \simeq \frac{1}{K} \sum_{i=1}^K A_i$$

How to generate equilibrium configurations?

Metropolis algorithm

(Metropoli-Rosenbluth-Rosenbluth-Teller-Teller=MR²T² algorithm)

- ▶ Sequence of configurations using a Markov chain
- ▶ Configuration is generated from the previous one
- ▶ Transition probability: equilibrium probability
- ▶ Detailed balance:

$$P(x)W(x \rightarrow x') = P(x')W(x' \rightarrow x)$$

- ▶ Rewritten:

$$\frac{W(x \rightarrow x')}{W(x' \rightarrow x)} = \frac{P(x')}{P(x)} = e^{-\beta \Delta E}$$

- ▶ Only the ration of transition probabilities are fixed

Metropolis algorithm

(Metropoli-Rosenbluth-Rosenbluth-Teller-Teller=MR²T² algorithm)

$$\frac{W(x \rightarrow x')}{W(x' \rightarrow x)} = \frac{P(x')}{P(x)} = e^{-\beta \Delta E}$$

► Metropolis:

$$W(x \rightarrow x') = \begin{cases} e^{-\beta \Delta E} & \text{if } \Delta E > 0 \\ 1 & \text{otherwise} \end{cases}$$

► Symmetric:

$$W(x \rightarrow x') = \frac{e^{-\beta \Delta E}}{1 + e^{-\beta \Delta E}}$$

Metropolis algorithm

Recipes:

- ▶ Choose an elementary step $x \rightarrow x'$ must be ergodic
- ▶ Calculate ΔE
- ▶ Calculate $W(x \rightarrow x')$
- ▶ Generate random number $r \in [0, 1]$
- ▶ If $r < W(x \rightarrow x')$ then new state is x' ; otherwise it remains x
- ▶ Increase time
- ▶ Measure what you want
- ▶ Restart

Movie1 Movie2

Metropolis algorithm, proposal probability

Transition probability:

$$W(x \rightarrow x') = g(x \rightarrow x')A(x \rightarrow x')$$

- ▶ $g(x \rightarrow x')$: proposal probability
 - ▶ Generally uniform
 - ▶ If different interactions are present then it must be incorporated
 - ▶ Generation method must be ergodic (reach all possible states)
- ▶ $A(x \rightarrow x')$: acceptance probability
 - ▶ Metropolis
 - ▶ Symmetric

Do we need optimization?

- ▶ Correlation length ξ
- ▶ Characteristic time τ_{char}
- ▶ Dynamical exponent z

$$\tau_{\text{char}} \propto \xi^z$$

- ▶ For 2d Ising model $z \simeq 2.17$
- ▶ Simulation time:

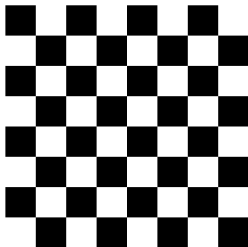
$$t_{\text{CPU}} \sim L^{d+z}$$

We need more effective algorithms!

Movie1 Movie2

Parallelization

- ▶ Observe that we have only local interaction
- ▶ For the update of a site we need the values of the four neighbors
- ▶ Nodes in a checkerboard structure can be updated in parallel
- ▶ can also be used for weak long range interactions



Cluster algorithm

- ▶ Flip more spins together. How?
- ▶ Transition probability:

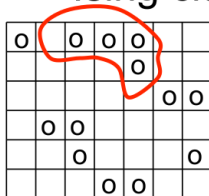
$$W(x \rightarrow x') = g(x \rightarrow x')A(x \rightarrow x')$$

- ▶ $g(x \rightarrow x')$: proposal probability
 - ▶ $A(x \rightarrow x')$: acceptance probability
- ▶ We used $g(x \rightarrow x') = 1$
- ▶ Can we have instead $A(x \rightarrow x') \equiv 1$?

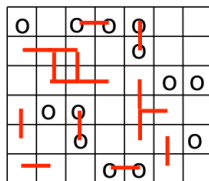
Cluster algorithm

- ▶ Flip more spins together. How?
 - ▶ The solution – based on an old relationship between the percolation and the Potts model – is that we consider the spin configuration as a correlated site percolation problem
 - ▶ Ising cluster: a percolating cluster of parallel spins
 - ▶ Ising droplets: a percolating subset of an Ising cluster
- $$p_B = 1 - \exp(-2\beta J)$$

Ising cluster



Ising configuration



Ising „droplets”

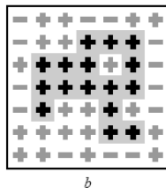
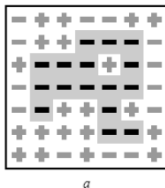
Swendsen-Wang algorithm

- ▶ Take an Ising configuration
- ▶ With probability $p_B = 1 - \exp(-2\beta J)$ make connection between *parallel* spins
- ▶ Identify the droplets by Hoshen-Kopelman algorithm
- ▶ Flip each droplet with probability: $1/2$ ($h = 0$)
- ▶ Repeat it over

Wolff algorithm

1. Add a random spin to a list of active spins
2. Take a spin from the active list
3. Add each parallel neighboring (not yet visited) spin with probability $p_B = 1 - \exp(-2\beta J)$ to the list of active spins
4. If list of active spins is not empty go to 2.
5. Flip all active spins

A Wolff droplet (gray)
before flipping



The new configuration
The droplet contour is
still shown, though the
bonds are eliminated
after flipping

Wolff algorithm *proof*

- ▶ Detailed balance:

$$P^{eq}(x)W(x \rightarrow x') = P^{eq}(x')W(x' \rightarrow x)$$

- ▶ Metropolis:

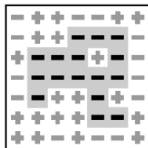
$$W(x \rightarrow x') = \min \left\{ 1, \frac{P^{eq}(x)}{P^{eq}(x')} \right\}$$

- ▶ Split W into acceptance A and proposal g probability

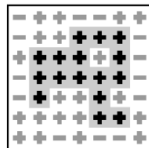
$$A(x \rightarrow x') = \min \left\{ 1, \frac{P^{eq}(x)g(x' \rightarrow x)}{P^{eq}(x')g(x \rightarrow x')} \right\}$$

Wolff algorithm *proof*

A Wolff droplet (gray)
before flipping



a



b

The new configuration
The droplet contour is
still shown, though the
bonds are eliminated
after flipping

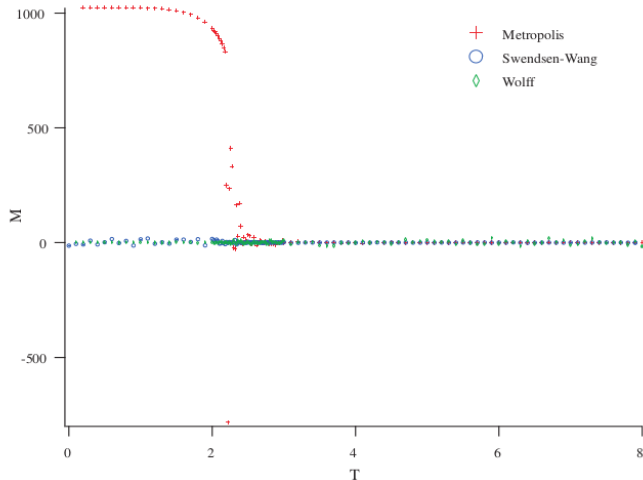
movie

- On the boundary: n_{same} spins parallel and n_{diff} antiparallel.

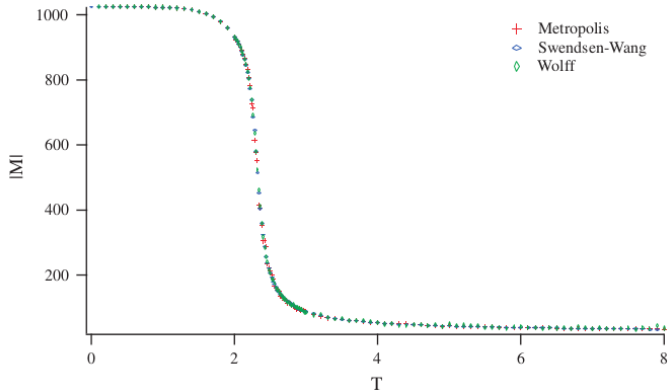
$$\begin{aligned} A(x \rightarrow x') &= \min \left\{ 1, \frac{e^{\beta J(n_{\text{diff}} - n_{\text{same}})}}{e^{\beta J(n_{\text{same}} - n_{\text{diff}})}} \frac{(1 - p_B)^{n_{\text{diff}}}}{(1 - p_B)^{n_{\text{same}}}} \right\} \\ &= \min \left\{ 1, \frac{e^{-2\beta J n_{\text{same}}}}{e^{-2\beta J n_{\text{diff}}}} \frac{(1 - p_B)^{n_{\text{diff}}}}{(1 - p_B)^{n_{\text{same}}}} \right\} \end{aligned}$$

- It gives: $p_B = 1 - \exp(-2\beta J)$.

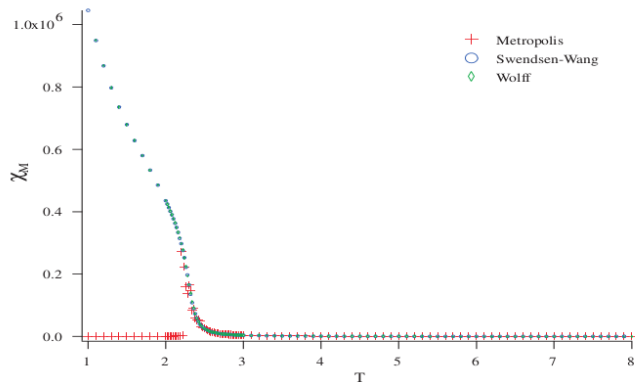
Comparison magnetization



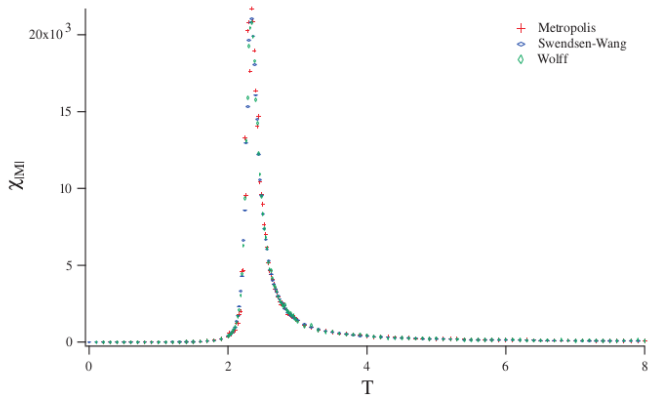
Comparison magnetization



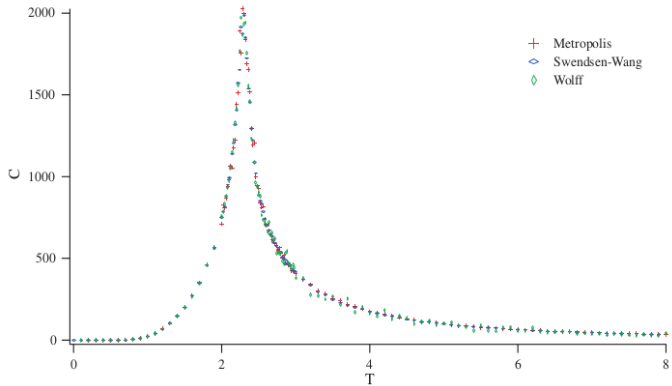
Comparison magnetization



Comparison magnetization



Comparison magnetization



Other ensembles

Microcanonical ensemble

- ▶ Daemon with bag with tolerance (both directions)
 - ▶ Pick a move, and calculate energy change
 - ▶ If energy change does not fit into bag reject it
 - ▶ Otherwise add energy change to bag
- ▶ In case of conservation the dynamic exponent z is larger!

Other ensembles

Conserved order parameter: Kawasaki dynamics

- ▶ Elementary step:
 - ▶ Exchange up-down spin pairs (can be anywhere) simultaneously
 - ▶ Apply Metropolis to net energy change!
 - ▶ Diffusive dynamics is more physical: pick neighboring spins
- ▶ In case of conservation the dynamic exponent z is larger!

Calculation of the entropy, free energy, etc.

- ▶ Equilibrium statistical physics: From F we can calculate everything
- ▶ In simulations F and S cannot be measured directly
- ▶ $F = E - TS$ so one of them is enough (E and T are known)
- ▶ Solution:
Calculate the specific heat!

$$C = k_B T^2 \langle (\Delta E)^2 \rangle$$

- ▶ The energy fluctuations are measurable
- ▶ Since

$$C = T \frac{\partial S}{\partial T}$$

We have

$$S(T) = S(T_0) + \int_{T_0}^T \frac{C(T')}{T'} dT'$$

Calculation of the entropy, free energy, etc.

- ▶ In many cases derivative of the entropy is needed so $S(T_0)$ is not important in

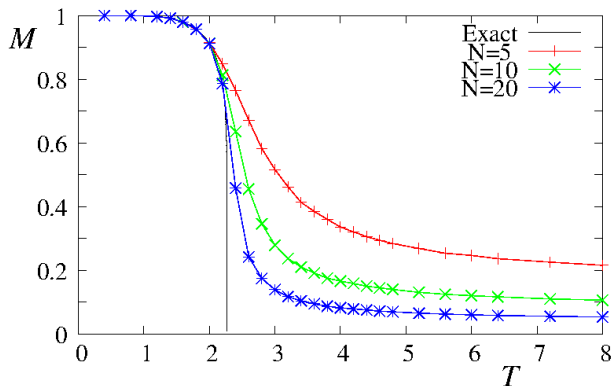
$$S(T) = S(T_0) + \int_{T_0}^T \frac{C(T')}{T'} dT'$$

- ▶ From third law of thermodynamics: $S(T = 0) = 0$.

Finite size effects

Magnetization 2d lattice Ising model

- Determine critical temperature
- Determine critical exponents
- System size dependence???



Finite size scaling

- ▶ Correlation length

$$\xi \propto |T - T_c|^{-\nu}$$

- ▶ Cannot be infinite!
- ▶ There will be a critical point for the finite system
- ▶ If L is finite ξ cannot be larger than L

$$L \propto |T(L) - T_c|^{-\nu}$$

- ▶ The position and the width of the transition

$$|T(L) - T_c| \propto L^{-1/\nu}$$

- ▶ 3 parameters to fit ν , T_c , and a constant

Finite size scaling

- ▶ Binder Cumulant method (find something which does not scale with L)
- ▶ Find something which scales with ν
 - ▶ The standard deviation of the order parameter:

$$\sigma(L) \propto L^{-1/\nu}$$

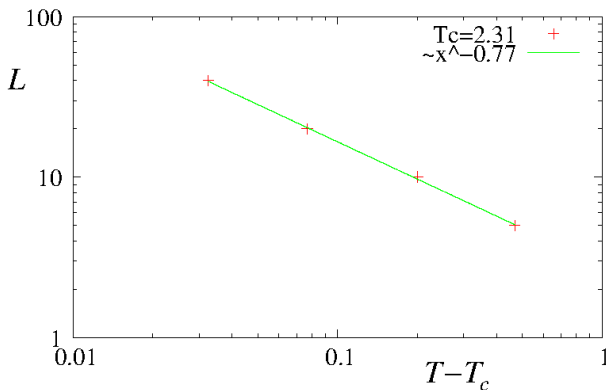
- ▶ Two steps, both with two parameter fits:

$$\sigma(L) \propto L^{-1/\nu}$$

$$|T(L) - T_c| \propto L^{-1/\nu}$$

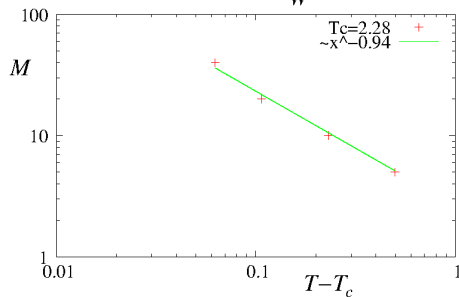
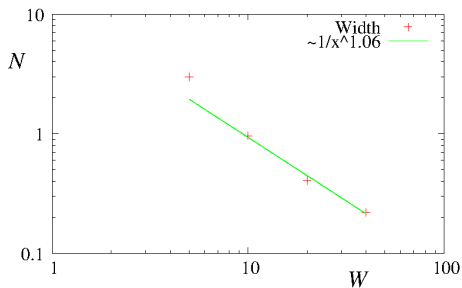
Three parameter fit: Ising model

- Theory: $\nu = 1$, $T_c \simeq 2.27$



Finite size scaling: Ising model

- Theory: $\nu = 1$, $T_c \simeq 2.27$



Variants

- ▶ Potts model:

- ▶ Spin is two dimensional unit vector with q possible values at angles

$$\theta_n = \frac{2\pi n}{q}$$

- ▶ Hamiltonian (vector, or clock model):

$$H_c = J_c \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$$

- ▶ Hamiltonian (standard):

$$H_p = -J_p \sum_{\langle ij \rangle} \delta(s_i, s_j)$$

- ▶ Results in two dimensions ($J>0$):
- ▶ First order phase transition for $q > 4$
- ▶ Second order phase transition for $q \leq 4$

Variants

- ▶ Classical XY model

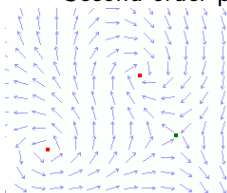
- ▶ Spin is two dimensional unit vector with θ_i angle

$$\mathbf{s}_i = (\cos \theta_i, \sin \theta_i)$$

- ▶ Hamiltonian:

$$H_{XY} = \sum_{\langle ij \rangle} J_{ij} \mathbf{s}_i \mathbf{s}_j$$

- ▶ Results in two dimensions ($J>0$):
 - ▶ Nearest neighbor interaction: No phase transition in 2d
 - ▶ Long range interaction ($J_{ij} \sim |\mathbf{r}_i - \mathbf{r}_j|^{-\alpha}$)
 - ▶ No phase transition
 - ▶ Kosterlitz-Thouless transition: Correlation function decays exponentially or as a power law
 - ▶ Second order phase transition in 3d



Variants

- ▶ Classical Hamilton model
 - ▶ Spin is **three** dimensional unit vector with θ_i angle
 - ▶ Hamiltonian:

$$H_H = \sum_{\langle ij \rangle} J_{ij} \mathbf{s}_i \mathbf{s}_j$$

- ▶ Similar results to XY model

Standard opinion models

- ▶ Would vote for *democrats/republicans*
- ▶ Can be represented by a spin
- ▶ One takes the opinion of the neighborhood majority
- ▶ Plus some noise
- ▶ This the Ising model
- ▶ More opinions than this is the Potts model with Hamming distance instead of cos

Voter model

- ▶ Spins/agents on a lattice (can be network)
- ▶ Spin can have q different values
- ▶ Interaction: copy one of the neighbors opinion
- ▶ Similar as Ising-model at temperatures slightly below the transition
- ▶ Note, that in social science nearest neighbors are the 8 surrounding sites
- ▶ Only domain boundaries are active
- ▶ Steady state a homogeneous system
- ▶ Convergence is slow $T(N) \sim N \log N$ in $d = 2$ and $T(N) \sim N$ in $d > 2$

Majority model

- ▶ Spins/agents on a lattice (can be network)
- ▶ Spin can have q different values
- ▶ Interaction: Select r neighbors (from 8 neighbors)
- ▶ If there is a majority opinion copy that
- ▶ Similar to Voter model

Synchronization



Synchronization



Kuramoto model

- ▶ Oscillator with angle θ_i

$$\frac{d\theta_i}{dt} = \omega_i + \frac{K}{N} \sum_{j=1}^N \sin(\theta_j - \theta_i)$$

- ▶ Two phases: Phase locking and random

MOVIE [Wikipedia](#)

Kuramoto model for 2 oscillators

- ▶ Two oscillators with own frequency ω_1, ω_2
- ▶ In general:

$$\frac{d\phi_1}{dt} = \omega_1 + H_{12}(\phi_1, \phi_2) \qquad \frac{d\phi_2}{dt} = \omega_2 + H_{21}(\phi_2, \phi_1)$$

- ▶ Kuramoto model:

$$\left. \begin{aligned} H_{12}(\phi_1, \phi_2) &= \frac{K}{2} \sin(\phi_2 - \phi_1) \\ H_{21}(\phi_2, \phi_1) &= \frac{K}{2} \sin(\phi_1 - \phi_2) \end{aligned} \right\} \frac{d\Delta\phi}{dt} = \Delta\omega - K \sin \Delta\phi$$

with

$$\Delta\phi = \phi_2 - \phi_1 \quad \Delta\omega = \omega_2 - \omega_1$$

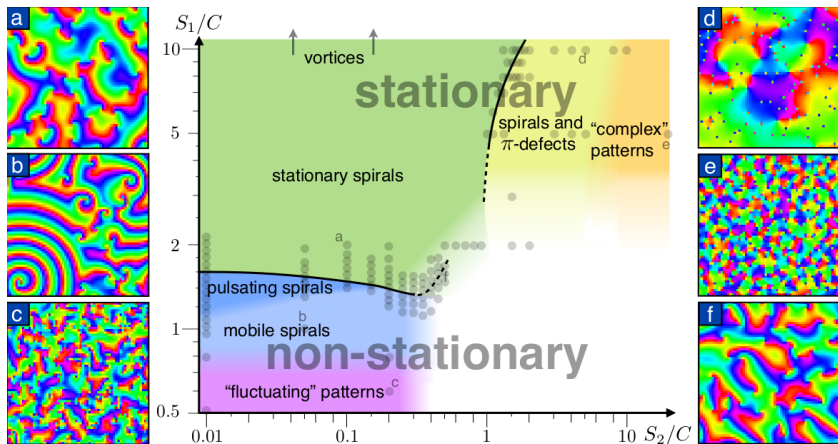
- ▶ Stationary solution:

$$\sin \Delta\phi = \frac{\Delta\omega}{K}$$

for

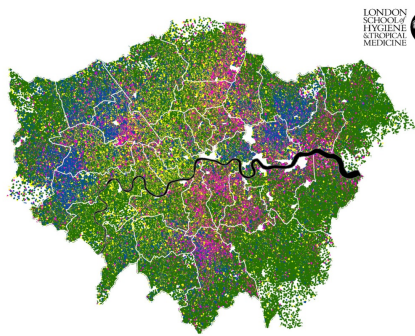
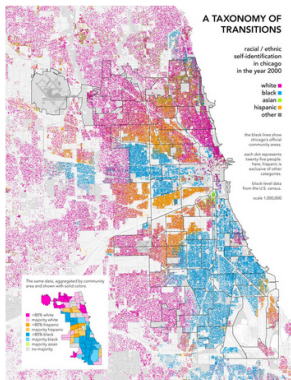
$$\left| \frac{\Delta\omega}{K} \right| \leq 1$$

Synchronization



Schelling model

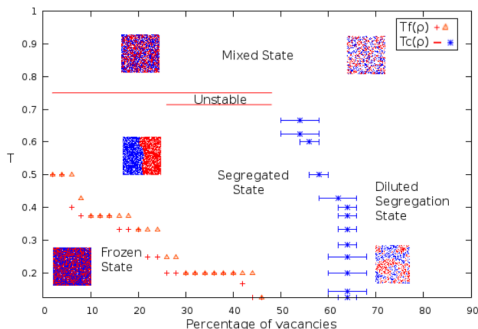
- Schelling model of segregation:
 1. Segregated neighborhoods reflect ethnic preferences of individuals
 2. Individual preferences reflect ethnic segregation.
 3. Is the answer “the chicken and the egg”?
 4. Or are both sides wrong?



■ : White- British ■ : White-Non-British ■ : Black or Black British ■ : Asian or Asian British

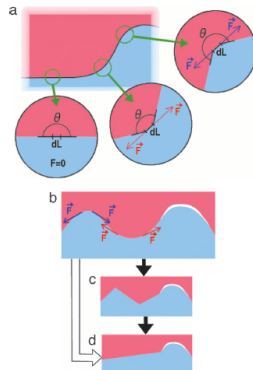
Schelling model

- ▶ Two equal-sized ethnic groups randomly distributed on a regular lattice
- ▶ Each agent has 8 neighbors 15% of cells are vacant
- ▶ If dissatisfied, agents pick the closest vacant slot that is satisfactory
- ▶ Dissatisfaction means that the fraction of alike neighbors is less than a parameter T
- ▶ Nobel prize in 2005



Schelling model

- ▶ In principle Ising model with conserved magnetization
- ▶ Only surface is important for the dynamics.
- ▶ Tolerance parameter sets minimal surface curvature (acts as surface tension)
- ▶ Surface curvature defines also volume/surface ratio which diverges easily



Practice

- ▶ Ising-model on a triangular lattice, with periodic boundary conditions

$$H = -J \sum_{\langle ij \rangle} s_i s_j$$

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

- ▶ On a triangular lattice the site i, j has the following six neighbors:
 - ▶ $(i+1, j), (i-1, j)$
 - ▶ If j is even: $(i-1, j \pm 1), (i, j \pm 1)$
 - ▶ If j is odd: $(i, j \pm 1), (i+1, j \pm 1)$
- ▶ Measure the global magnetization, and the energy fluctuation
- ▶ Use small systems $L = 5, 10, 20$ and $T \simeq 0.1 - 10$
- ▶ (Bonus for extra points) Do the finite size scaling

Triangular lattice

