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:

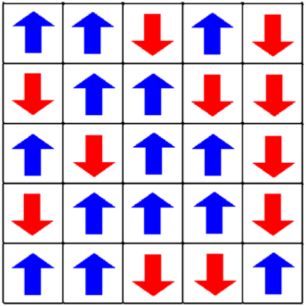
$$H(\sigma) = -\sum_{\langle i\ j \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_i h_i\sigma_i$$

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

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

- In the canonical ensemble

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

- 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=MR^2T^2 algorithm)

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

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

- Rewritten:

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

- Only the ration of transition probabilities are fixed

Metropolis algorithm

(Metropoli-Rosenbluth-Rosenbluth-Teller-Teller=MR^{2}T^2 algorithm)

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

- Metropolis:

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

- Symmetric:

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

Metropolis algorithm

Recipes:

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

Movie1

Metropolis algorithm, proposal probability

Transition probability:

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

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

Do we need optimization?

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

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

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

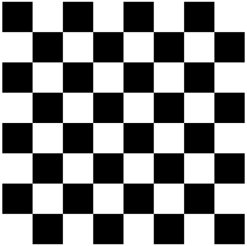
$$t_{\mathrm{CPU}} \sim L^{d+z}$$

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

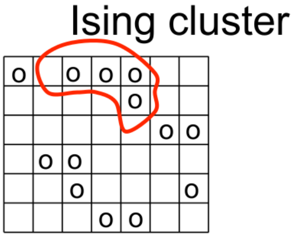
- Flip more spins together. How?
- Transition probability:

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

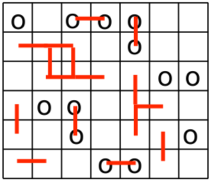
  - $g(x \to x')$: proposal probability
  - $A(x \to x')$: acceptance probability
- We used $g(x \to x') = 1$
- Can we have instead $A(x \to x') \equiv 1$?

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 configuration



Ising „droplets”

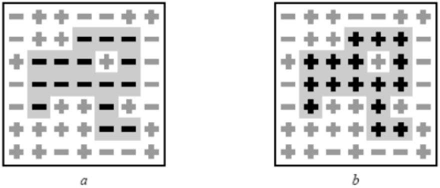
Swendsen-Wang algorithm

- 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:

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

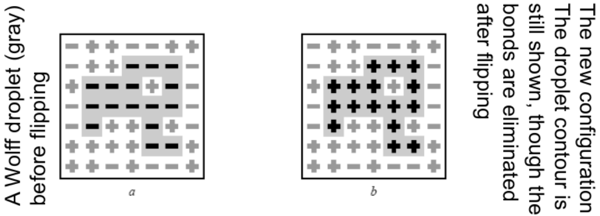
- Metropolis:

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

- Split W into acceptance A and proposal g probability

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

Wolff algorithm *proof*



movie

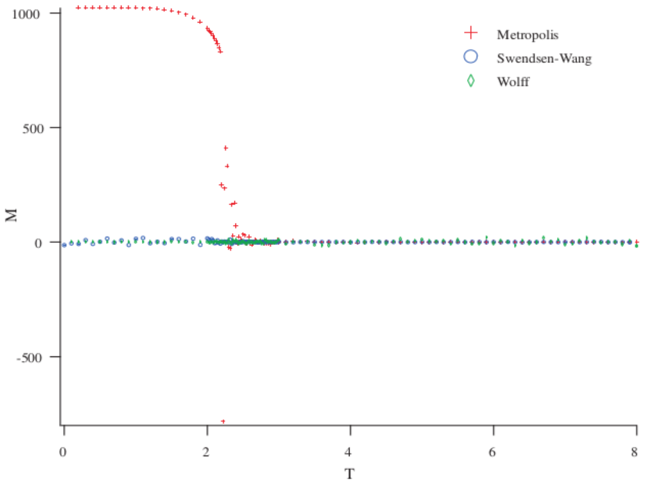
- On the boundary: n_{same} spins parallel and n_{diff} antiparallel.

$$A(x \to x') = \min\left\{1, \frac{e^{\beta J(n_{\text{diff}} - n_{\text{same}})}}{e^{\beta J(n_{\text{same}} - n_{\text{diff}})}} \frac{(1-p_B)^{n_{\text{diff}}}}{(1-p_B)^{n_{\text{same}}}}\right\}$$

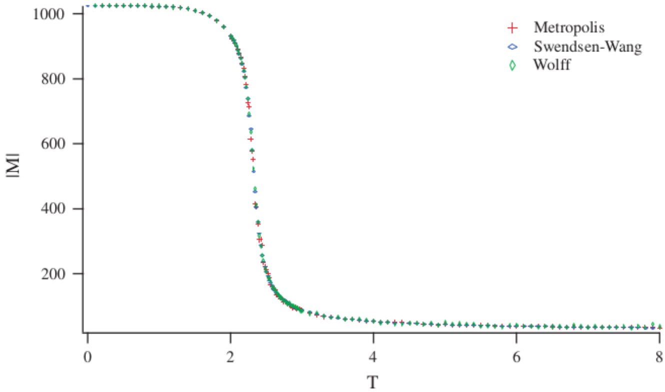
$$= \min\left\{1, \frac{e^{-2\beta J n_{\text{same}}}}{e^{-2\beta J n_{\text{diff}}}} \frac{(1-p_B)^{n_{\text{diff}}}}{(1-p_B)^{n_{\text{same}}}}\right\}$$

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

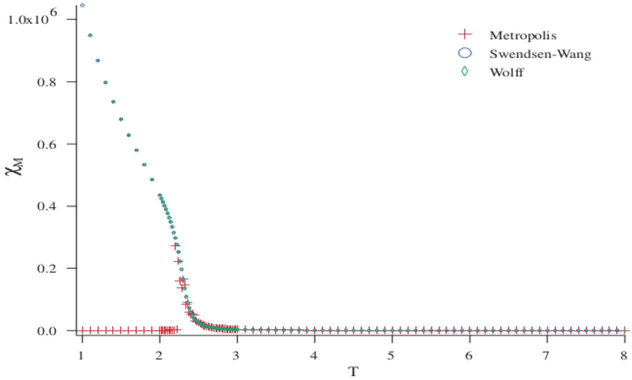
Comparison magnetization



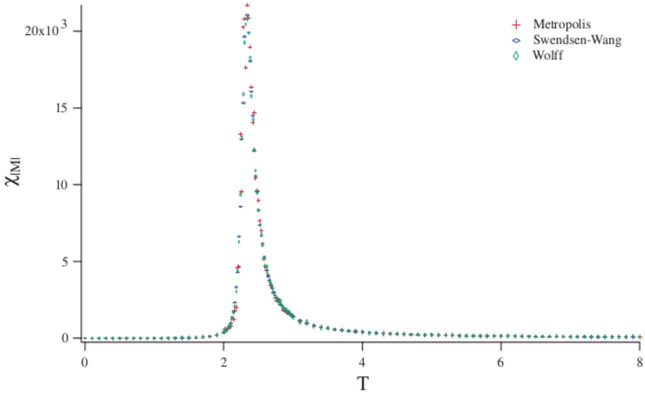
Comparison magnetization



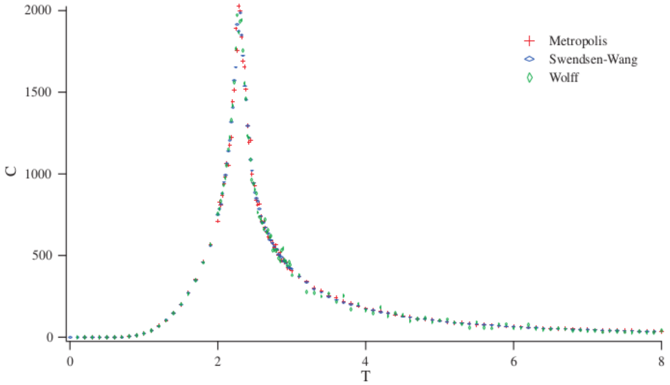
Comparison magnetization



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

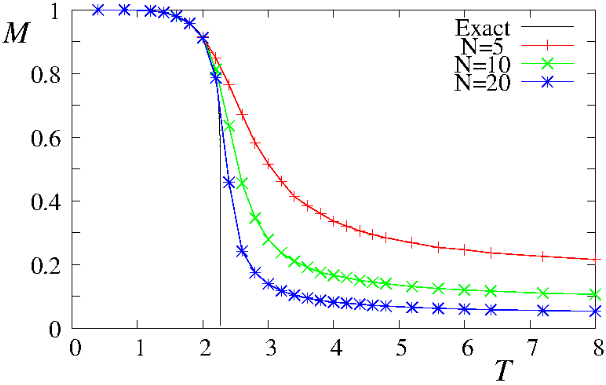
$$S(T) = S(T_0) + \int_{T_0}^{T} \frac{C(T')}{T'} dT'$$

- 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:

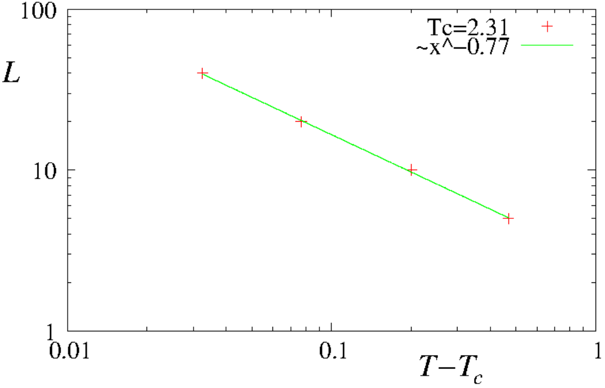
$$\sigma(L) \propto L^{-1/\nu}$$

  - Two steps, both with two parameter fits:

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

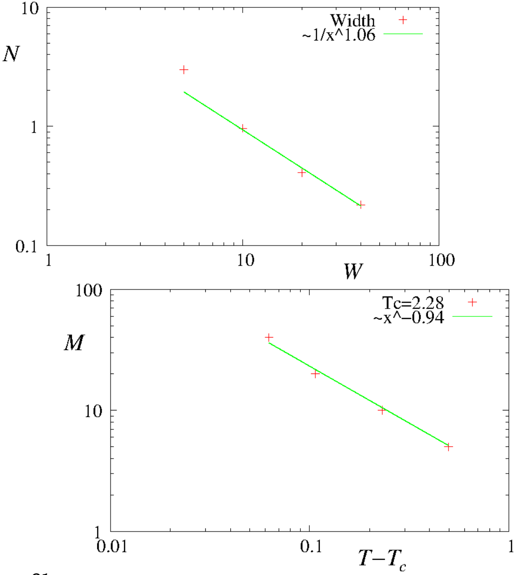
Three parameter fit: Ising model

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



Finite size scaling: Ising model

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

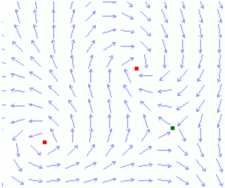


Variants

- 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 $q <= 4$

Variants

- Classical XY model
  - Spin is two dimensional unit vector with θ_i angle
    $$\mathsf{s}_i = (\cos\theta_i, \sin\theta_j)$$
  - Hamiltonian:
    $$H_{XY} = \sum_{\langle ij \rangle} J_{ij} \mathsf{s}_i \mathsf{s}_j$$
  - Results in two dimensions (J>0):
  - Nearest neighbor interaction: No phase transition in 2d
  - Long range interaction ($J_{ij} \sim |\mathsf{r}_i - \mathsf{r}_j|^{-\alpha}$)
    - No phase transition
    - Kosterlitz-Thoughless transition: Correlation finctuion 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:
$$H_H = \sum_{\langle ij \rangle} J_{ij} \mathsf{s}_i \mathsf{s}_j$$
  - 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:

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

with

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

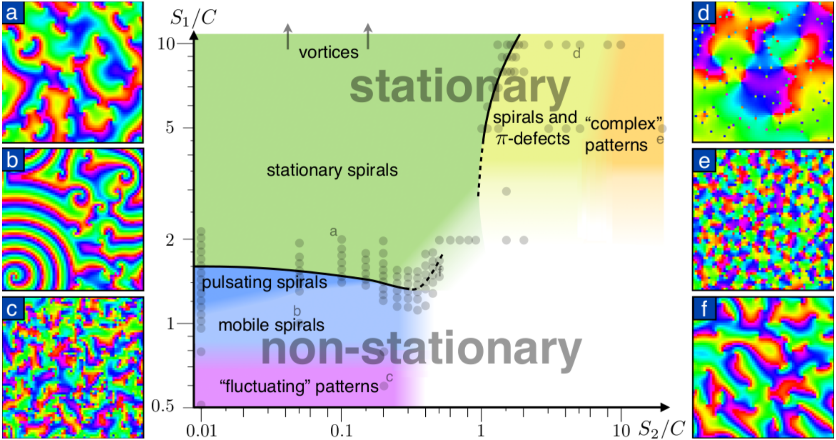
- Stationary solution:

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

for

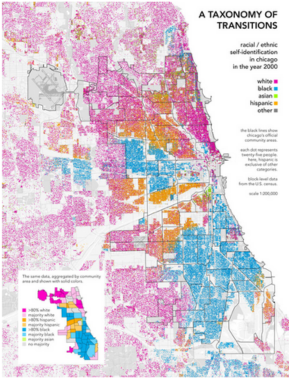
$$\left|\frac{\Delta\omega}{K}\right| \leq 1$$

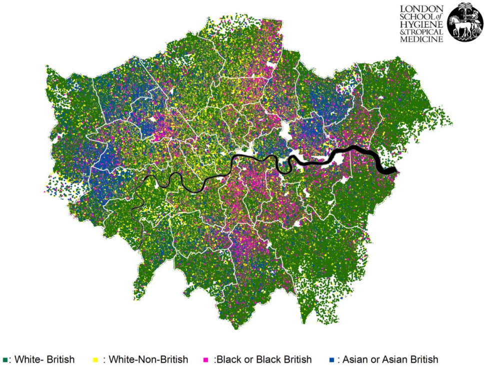
Synchronization



Schelling model

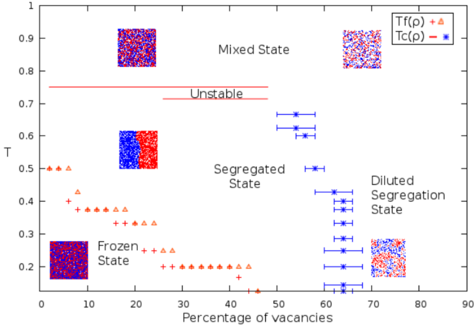
- Schelling model of segregation:
  1. Segregated neighborhoods reflect ethnic preferences of individuals
  2. Individual preferences reflect ethnic segregation.
  3. Is the answer “the chicken and the egg”?
  4. Or are both sides wrong?





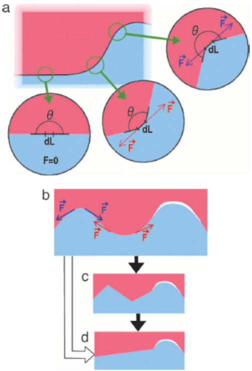
Schelling model

- 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

- Choose one of the following:
- Simulate Ising-model in three dimensions with periodic boundary conditions
  - The Hamiltonian
    $$H = -J \sum_{\langle ij \rangle} s_i s_j$$
    where $s_i \in \{-1, +1\}$, sum runs for the 8 neighbors
  - 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
- Simulate the Schelling model
  - There are three parameters: L, T, fraction of vacant sites
  - Start from random configuration
  - Identify dissatisfied agents (empty houses does not count!)
  - Move dissatisfied agents to a random empty space
  - Stop if everybody is satisfied or enough time is lapsed