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

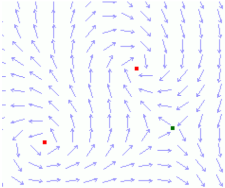
$$M = \sum_i \sigma_i$$

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
    $$\mathrm{s}_i = (\cos\theta_i, \sin\theta_j)$$
  - Hamiltonian:
    $$H_{XY} = \sum_{\langle ij\rangle} J_{ij}\mathrm{s}_i\mathrm{s}_j$$
  - Results in two dimensions (J>0):
  - Nearest neighbor interaction: No phase transition in 2d
  - Long range interaction ($J_{ij} \sim |\mathrm{r}_i - \mathrm{r}_j|^{-\alpha}$)
    - 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

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

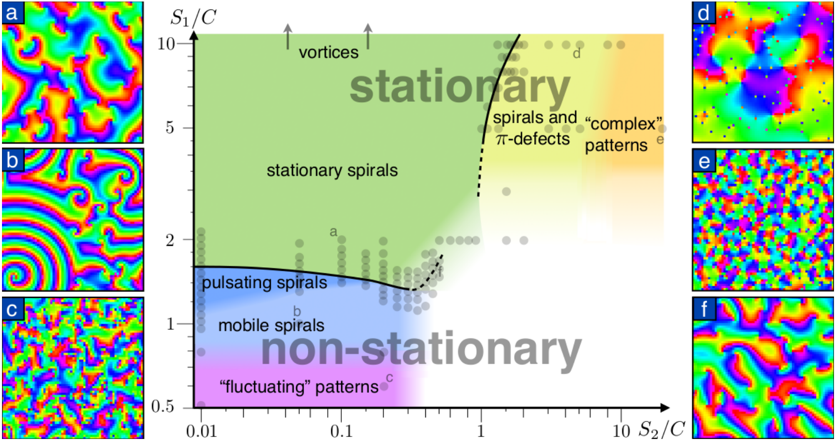
- Stationary solution:

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

  for

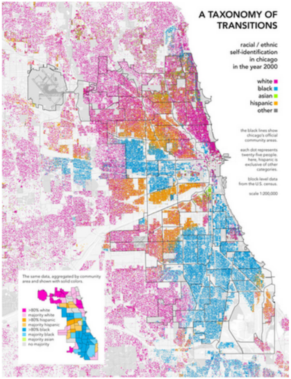
$$\left|\frac{\Delta\omega}{K}\right| \leq 1$$

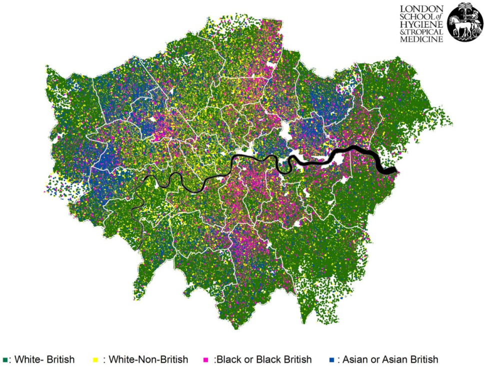
Synchronization



Schelling model

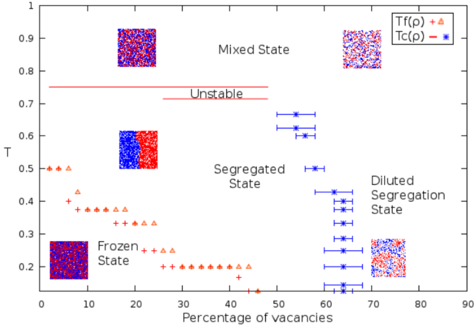
- Schelling model of segregation:
    1. Segregated neighborhoods reflect ethnic preferences of individuals
    2. Individual preferences reflect ethnic segregation.
    3. Is the answer "the chicken and the egg"?
    4. Or are both sides wrong?





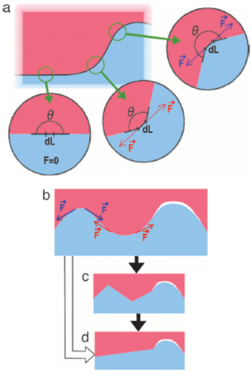
Schelling model

- 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

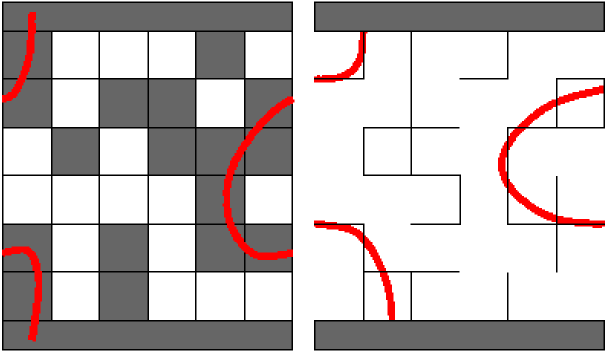


Percolation

Percolation

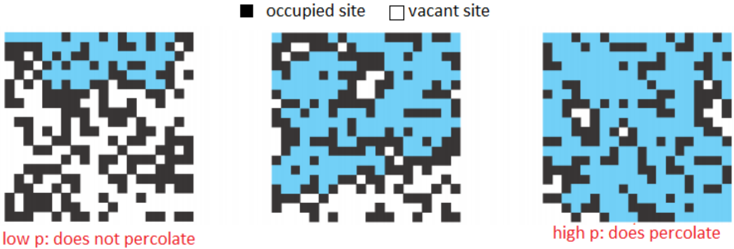
Behavior of connected cluster

- Site percolation
- Bond percolation



Percolation model

- Random environment
- With probability p site vacant (conducts)
- Two states: percolates or not!



Percolation theory

Questions (in infinite systems):

1. Is there an infinite cluster in infinite systems?
2. How many infinite clusters are there?
3. Mean cluster size (without the infinite one)?
4. Cluster size distribution

Answers:

1. Above a critical density with probability 1 below it with probability 0
2. Only 1!
3. Decreases as a power low away from the critical density
4. Power law

Percolation theory

Questions (in infinite systems):

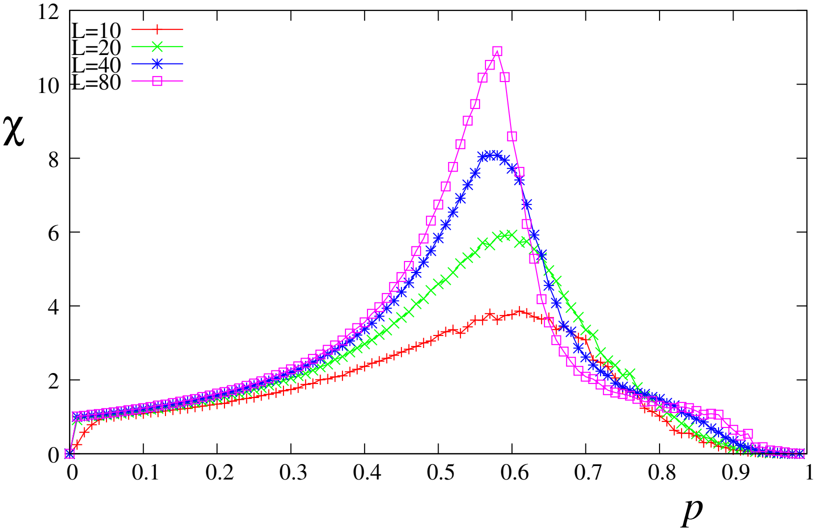
1. Is there an infinite cluster in infinite systems?
2. How many infinite clusters are there?
3. Cluster size distribution (n_s)
4. Mean cluster size (without the infinite one)? ($S = \sum_s s^2 n_s$)

Answers:

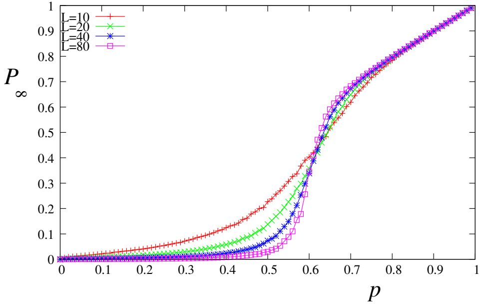
1. if $p > p_c$ then yes, otherwise no
2. Only 1!
3. $n_s \sim s^{-\tau}$
4. $S \sim |p - p_c|^{-\gamma}$

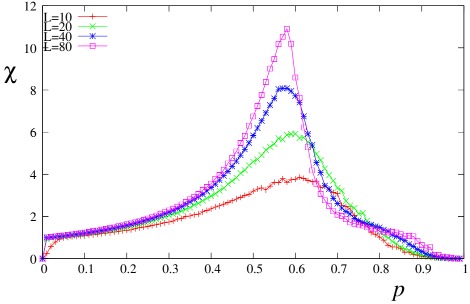
Like a second order phase transition in a geometric system!

Percolation model

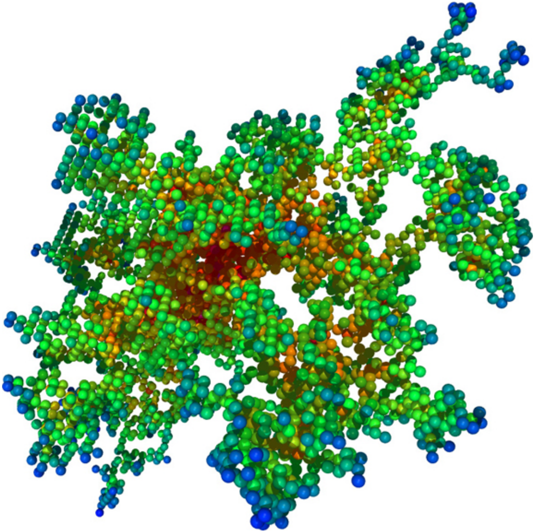


Percolation model

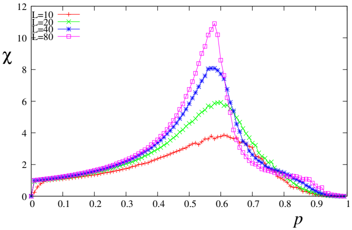


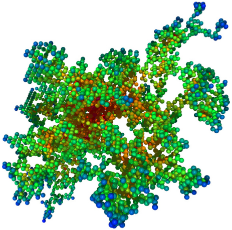


Percolation model



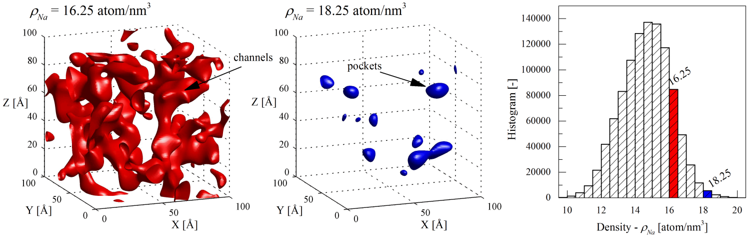
Percolating cluster

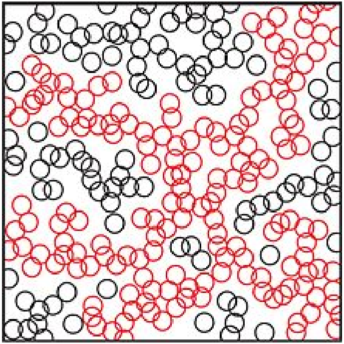


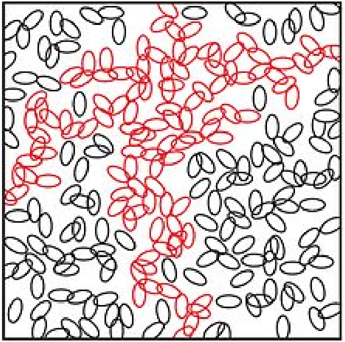


- Largest cluster
  - fractal with fractal dimension of d_f
  - $S_\infty \sim \begin{cases} \xi_f^d \log(N/\xi^d) & p < p_c \\ N^{d_f/d} & p = p_c \\ NP_\infty(p) & p > p_c \end{cases}$
- Largest not infinite cluster: size $\sim |p - p_c|^{-\nu}$

Percolation theory: Importance







Percolation theory: Importance

- COFFEE!!!!
- Non-equilibrium statistical physics
- Image analysis
- Percolation on networks: Phase transitions
- Percolation on networks: robustness, fragility
- Flooding

Percolation model

Bond [site] percolation

- Let us have a lattice (network)
- Each bond [site] is occupied with probability p
- (unoccupied with probability $1 - p$)
- A cluster is a set of sites connected by occupied bonds
  [A cluster is a set of occupied sites]

Hoshen-Kopelman Algorithm

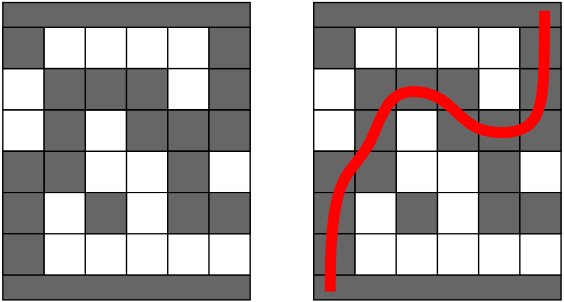
- Numerical task: find clusters
- Identify clusters
- Visit all sites
- Mark them with numbers

1	0	1	1	0	0	1	1	1	1	1	1	1	1	0
0	0	1	0	0	1	0	0	1	1	1	0	0	0	1
0	1	1	1	1	0	0	0	0	1	0	1	1	1	1
1	0	1	1	0	1	0	0	0	0	1	1	0	0	1
0	0	1	1	0	0	0	0	1	0	0	0	1	0	1
1	0	1	0	1	0	0	0	1	0	0	1	0	1	1
1	1	0	0	1	0	1	1	1	1	1	1	1	1	0
1	0	0	1	1	1	0	0	1	1	1	0	0	1	1
1	1	0	1	1	1	0	1	0	1	0	0	1	0	0
0	0	1	0	0	1	1	0	1	1	0	1	1	0	0

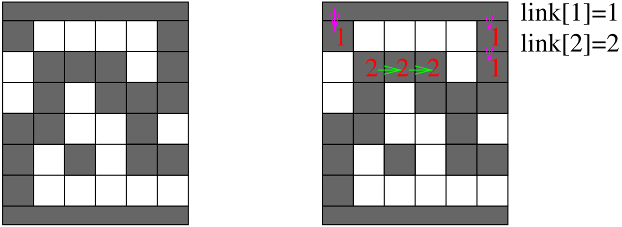
1	0	2	2	0	0	3	3	3	3	3	3	3	3	0
0	0	2	0	0	4	0	0	3	3	3	0	0	0	5
0	2	2	2	2	0	0	0	0	3	0	5	5	5	5
6	0	2	2	0	7	0	0	0	0	5	5	0	0	5
0	0	2	2	0	0	0	0	5	0	0	0	8	0	5
9	0	2	0	10	0	0	0	5	0	0	5	0	5	5
9	9	0	0	10	0	5	5	5	5	5	5	5	5	0
9	0	0	10	10	10	0	0	5	5	5	0	0	5	5
9	9	0	10	10	10	0	11	0	5	0	0	12	0	0
0	0	13	0	0	10	10	0	5	5	0	12	12	0	0

Hoshen-Kopelman Algorithm

- Site percolation
- Open boundary conditions
- Go through site in typewriter style
- Check left and above

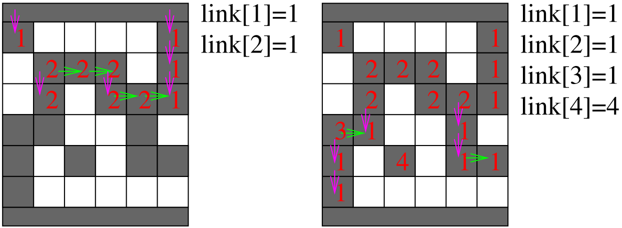


Hoshen-Kopelman Algorithm



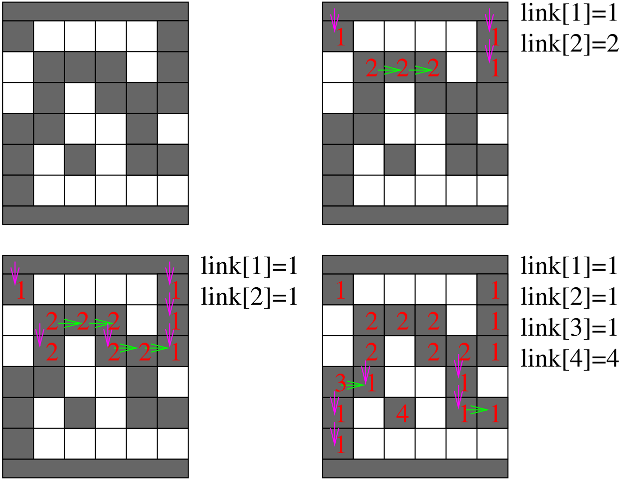
- Go through sample in typewriter style
- If site is occupied, look left and up
  - if no neighbour → new number
  - if only one is occupied → inherit number

Hoshen-Kopelman Algorithm



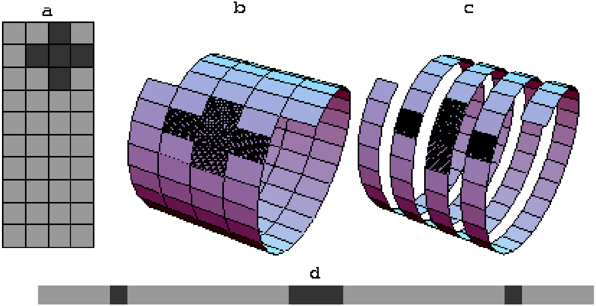
- ...
- If site is occupied, look left and up
  - ...
  - if both sites are occupied $\rightarrow$ then link the two
    - a link which points to itself is a root link
    - find the root of both sites
    - connect the larger to the smaller
    - use this number

Hoshen-Kopelman Algorithm



Hoshen-Kopelman Algorithm

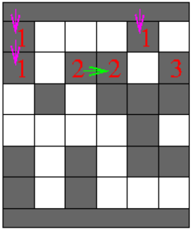
- Site percolation
- Helical boundary conditions (rolled up ont dimensional lattice)
- Go through site in typewriter style
- Check left and above (as before)



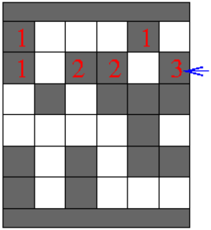
Hoshen-Kopelman Algorithm

- Site percolation
- Periodic boundary conditions
- Go through site in typewriter style
- Check left and above (as before)
- After each line if first and last site is occupied link them

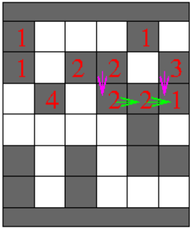
Hoshen-Kopelman Algorithm, Periodic BC



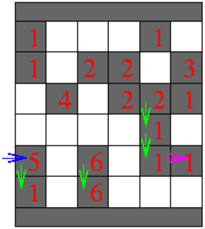
link[1]=1
link[2]=2
link[3]=3



link[1]=1
link[2]=2
link[3]=1

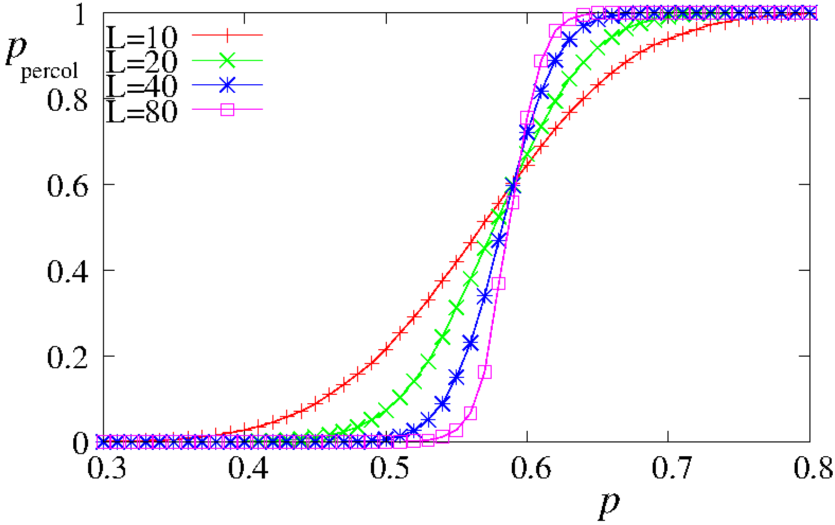


link[1]=1
link[2]=1
link[3]=1
link[4]=4



link[1]=1
link[2]=1
link[3]=1
link[4]=4
link[5]=1
link[6]=6

Result



Practice: Hoshen-Kopelman Algorithm

- Fill a square lattice by 1 with probability p and by 0 otherwise
- Create a large enough array where `link[i]=i`
- Write a root finding function which recursively sets `i` $\leftarrow$`link[i]` until `i == link[i]`
- Go through the lattice in a typewriter style
- If the site is not empty check the sites to the top and left (if they exist)
  - if both neighbors are empty $\rightarrow$ assign it a new label (you can keep the labels in the original array)
  - if only one neighbor is empty $\rightarrow$ assign it the root label of the neighbor
  - if both neighbors are occupied $\rightarrow$ search for the root labels of the sites connect the larger to the smaller and assign this value to this site
- (Bonus): Measure the distribution of the size of the clusters, or the size of the largest as function of p, etc.

Practice

Simulate the Schelling model

- There are three parameters: L, T, fraction of vacant sites
- Start from random configuration
- Agents have 8 neighbors
- 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