Simulations in Statistical Physics

Course for MSc physics students

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Homework 1

Wolff cluster algorithm Responsible: Gábor Mándi

Write a program that uses the Wolff cluster algorithm for the Ising model on the three-dimensional cubic lattice!

- Determine the spontaneous magnetization and the susceptibility as a function of the temperature and system size.
- Apply finite size scaling to the problem, use $L = 4,\ 8,\ 16$.

Homework 2

2D diffusion-limited aggregation. Responsible: György Vida

Write a computer simulation of the two-dimensional diffusion-limited aggregation model on triangular and square lattices: Introduce your own measure of anisotropy parameter and determine the difference between the two lattices. Measure the fractal dimension.

Homework 3

Epidemic model on ER graph Responsible: László Ujfalusi

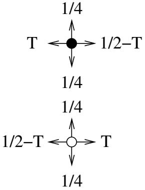
Generate an Erdős-Rényi graph with fixed $\langle k \rangle = 3$. Investigate the following epidemic model on this network:
There are three kinds of nodes: susceptible (**S**), infected (**I**), recovered (**R**). In every time step an infected node infects its susceptible neighbours with probability β, infected sites can recover with probability γ. A recovered site cannot become infected again, and they do not infect any susceptible site.
In the beginning every site is susceptible, except for 10 which are infected. Using the system size $N = 1000$, $\gamma = 0.1$ show that the limit for the infection to grow is $\beta > \gamma/\langle k \rangle$. Use ensemble averages!

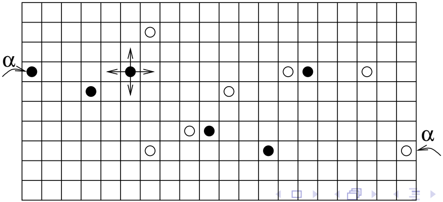
Homework 4

Dynamical Monte Carlo simulation Responsible: Balázs Nagyfalusi

Simulate a lattice gas with Monte Carlo method. The lattice is 20x10 sites and is periodic in the vertical direction. There are two type of particles: black and white ones. Black ones are inserted on the left hand side of the lattice with rate α (choose a site, if it is empty put there a black particle with probability α.) White particles are inserted on the right side with the same rate. Particles which leave either left or right the lattice are discarded.

The particles may move to *empty* adjacent sites with the probabilities shown on the figure. Measure (ensemble average) the current and the density in function of α and $T \in [0, 1/2]$.





Homework 5

Page-Rank on BA network Responsible: Grörgy Vida

Create a directed Barabási-Albert network with $m = 2$. Start with a triangle. When a new node is added it has two outgoing link which is attached to a node j with probability proportional to k_j, where k_j is the degree of the node including both the incoming and outgoing links. For $N = 100$ calculate the *page rank* and plot the degree-PageRank and age=PageRankcorrelation. (Use ensemble average, perform the simulation on different realizations of the graph.)

Homework 6

Ising spin glass with genetic algorithm Responsible: Levente Rózsa

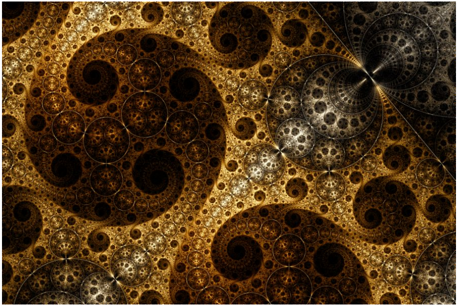
Consider an $N \times N$ square lattice with periodic boundary conditions and the Hamiltonian

$$H = -\sum_{<i,j>} J_{ij} s_i s_j .$$

The summation goes over the nearest neighbour pairs. The J_{ij} coupling coefficients are randomized at the start of the simulation by setting them to ± 1 with probability 0.5. The $s_i = \pm 1$ variables represent the Ising spins at the lattice points. Determine the approximate ground state energy per lattice point in the system by using a genetic algorithm, with the set of s_i values on the lattice as the genetic code.

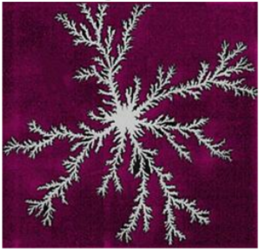
Use a set of P different realizations, for the next generation choose $P/2$ with the lowest energies. Generate $P/2$ random children with random gene mixing. Two random genes of individuals get mutated with probability $p = 1/4$. Use $N = 8,\ 16$ and $P = 100,\ 200,\ 400.$

Fractals



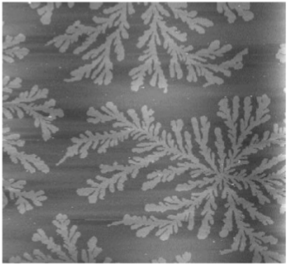
Fractal growth

Fractal growth



Elctrochem. deposition

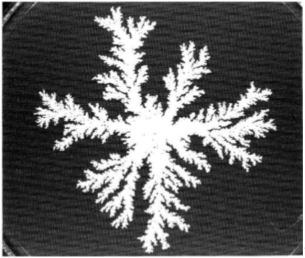
Mineralization



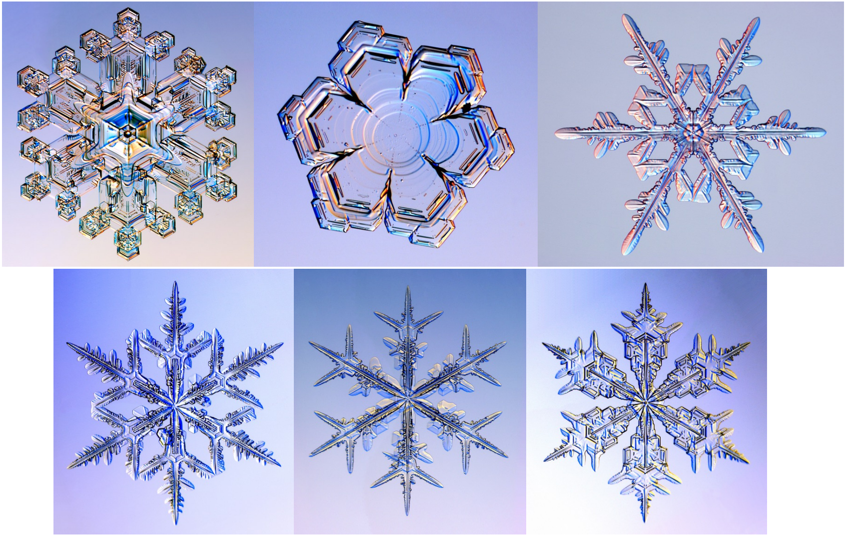
Surface crystallization

Disordered viscous fingering

Bacterial colony growth



Snowflakes



Fractal growth

Laplacian or gradient governed growth

- Scalar field (electrostatic field, density, through diffusion)

$$\Delta u = 0$$

- Velocity of the interface Γ proportional with the gradient

$$\mathbf{v}|_\Gamma = -C \nabla u|_\Gamma$$

- Boundary condition: potential is curvature (κ) dependent

$$u|_\Gamma = f(\nabla u, \kappa)$$

- Disorder: small fluctuations

Fractal growth

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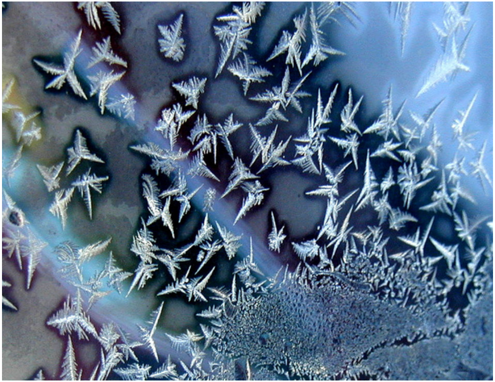


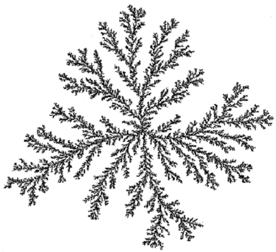
Fractal growth

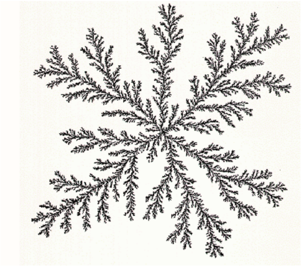
Consequences:

- *Positive growth feedback*: If there is a bump, gradient increases (peak effect), growth gets faster
- *Screening*: Faster bump will screen the slower one
- *Branching*: If tip is far a new bump may grow.
- *Tip splitting*: Tip gets instable and splits

Fractal

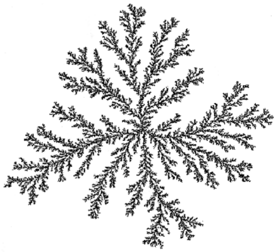
- Self-similarity
- Repeating pattern
- Scaling patterns

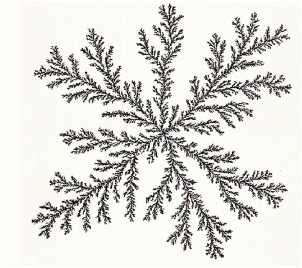




Diffusion Limited Aggregation

- Starting from a seed
- Particles come from infinity with diffusion
- If incoming particle touches cluster it gets stuck to it
- Samples: 1m and 100m particles





Diffusion Limited Aggregation: Algorithm

Basic:

- Start with a seed at (0,0)
- Particles start far from the aggregate and diffuse till they get adjacent to existing cluster

Advanced:

- Start with a seed at (0,0)
- Start random walker on a circle just big enough to cover the cluster
- Define a kill ring big enough or use reentry distribution
- Regions of large jumps, on a larger scale lattice

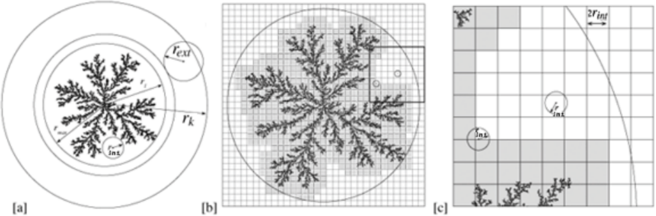


FIG. 1: (a) Schematic representation of the "optimized random trajectories". (b) A DLA aggregate and a mesh of cells $2r_{int} \times 2r_{int}$. Long steps are forbidden in the gray boxes and allowed in the white ones. Also, two long steps are illustrated. (c) A zoom of the region inside the large square in (b).

Diffusion Limited Aggregation: Algorithm

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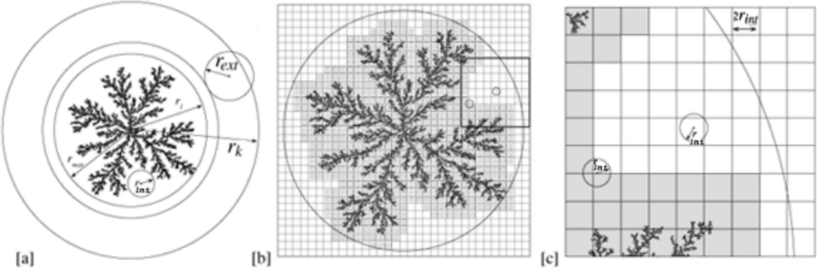
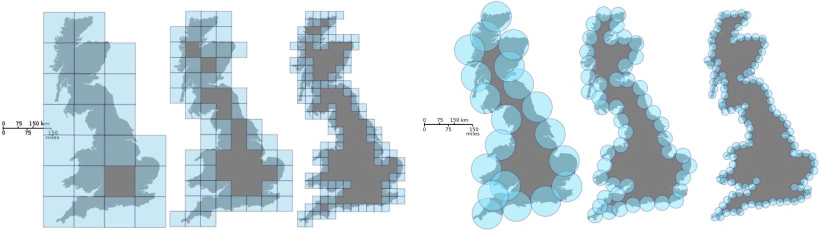
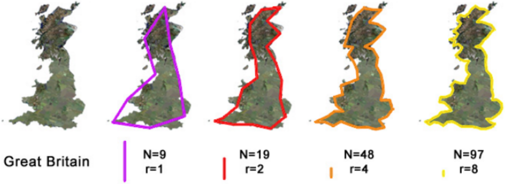


FIG. 1: (a) Schematic representation of the "optimized random trajectories". (b) A DLA aggregate and a mesh of cells $2r_{int} \times 2r_{int}$. Long steps are forbidden in the gray boxes and allowed in the white ones. Also, two long steps are illustrated. (c) A zoom of the region inside the large square in (b).

Dimension

- $d = 0$ point, $d = 1$ line, $d = 2$ plane, etc. Containing space.
- Dimension of a finite object: Cover it
- Hausdorff (fractal) dimension
- Minkowski–Bouligand dimension





Fractal dimension

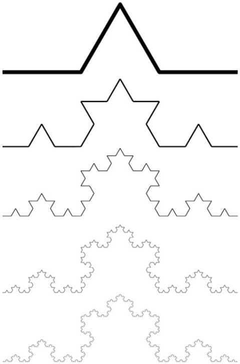
- Fractal dimension
  - Cover the object with boxes of size ε, the fractal dimension is:

$$D = \dim(S) \equiv \lim_{\varepsilon \to 0} \frac{\log N(\varepsilon)}{\log 1/\varepsilon}$$

- Differences:
  - Minkowski–Bouligand: Regular lattice is used
  - Hausdorff: Spheres of given size are used.
- In practice

$$N(\varepsilon) \propto \varepsilon^D$$

Fractal dimension: Example



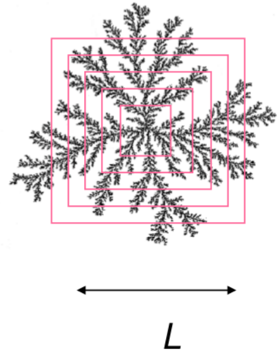
Koch curve

- Start from unit segment
- Hausdorff dimension: cover it with spheres of size $l = 3^{-i}$
- Number of spheres needed $N_l = 4^i$ (take level i!)
- Fractal dimensions:

$$D = \frac{\log N_l}{\log 1/l} = \frac{i \log(4)}{+i \log(3)} = \log_3(4)$$

Fractal dimension: Other methods

- Sandbox method: $M \propto L^D$



- Correlation functions

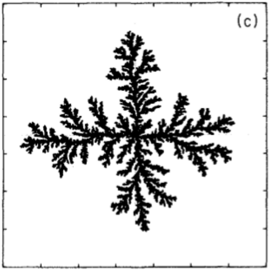
$$C(r) = \langle \rho(r)\rho(0) \rangle \propto r^{-\alpha}$$

$$D = d - \alpha$$

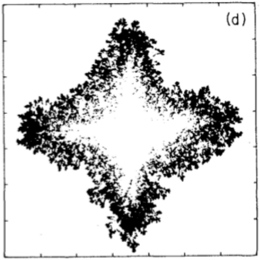
DLA: Lattice effects

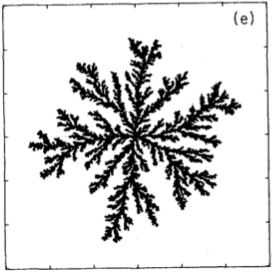
10^6 particles

10 clusters of 10^5 particles

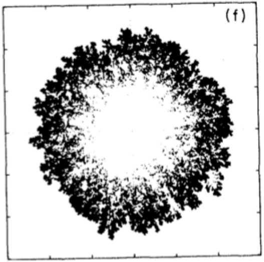


on-lattice





off-lattice

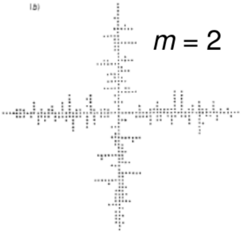


DLA: Lattice effects

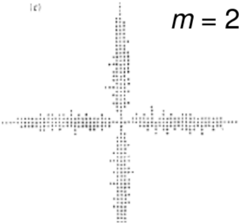
DLA on a lattice is anisotropic but splitting tips are observed!
Randomness suppresses the stabilizing effect.

No much difference between lattice and off lattice DLA (a)

What if we suppress randomness?
„Noise reduction": The growth happens only after the m-th particle arrives at the growth site. Ordinary DLA: m=1

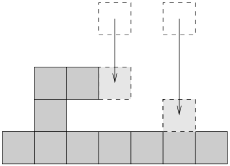


$m = 2$

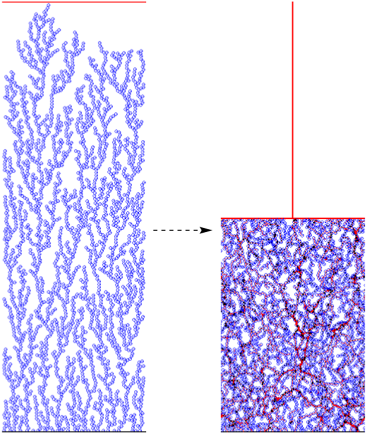


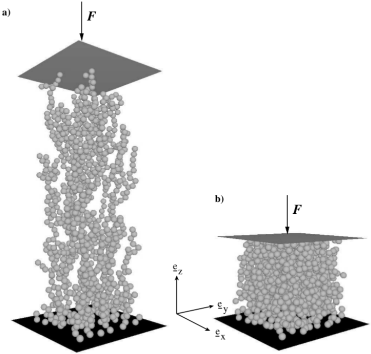
$m = 20$

Ballistic deposition



- Lattice
- Off lattice

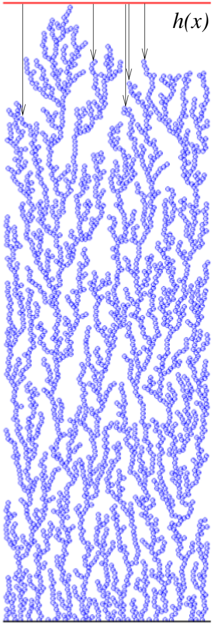




Surface growth models

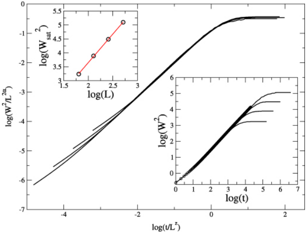
- Not the whole object but only its surface is interesting (e.g. coastline)
- Object starts from a d-dimensional substrate
- Object grows in the $d+1$th dimension.
- Object is described by $h(\mathbf{x})$ ($\mathbf{x}$ is a d-dimensional position vector) height function which is the maximum surface position at $\mathbf{x}$.
- Width of the surface

$$w(L,t) = \sqrt{\frac{1}{L}\int_0^L [h(x,t) - \bar{h}(t)]^2 dx}$$



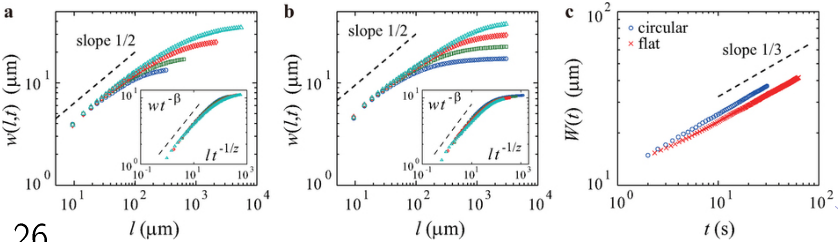
Family-Vicsek scaling

- Change of width in time



- Scaling relation:

$$w(L,t) \propto L^{\alpha} f(t/L^{z})$$



Theory: The KPZ-equation

- Surface growth $\dot{h}(\mathbf{x}, t)$
- Function of: position(?), height, gradient, Laplace of height, noise

$$\dot{h}(\mathbf{x}, t) = f[\mathbf{x}, h(\mathbf{x}, t), \nabla h(\mathbf{x}, t), \Delta h(\mathbf{x}, t), \ldots, \eta(\mathbf{x}, t)]$$

- Normally:

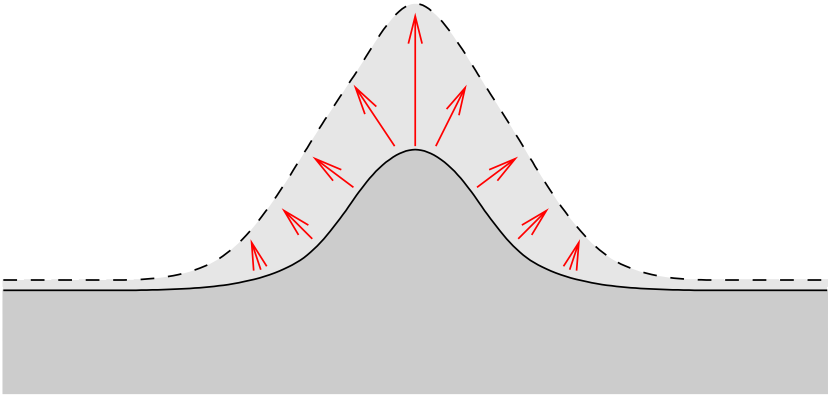
$$\dot{h}(\mathbf{x}, t) = f[h(\mathbf{x}, t), \nabla h(\mathbf{x}, t), \Delta h(\mathbf{x}, t), \eta(\mathbf{x}, t)]$$

- Gaussian noise:

$$\langle \eta(\mathbf{x}, t)\eta(\mathbf{x}', t')\rangle = A\delta(t - t')\delta(x - x')$$

$$P(\eta) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{\eta^2}{2\sigma}\right)$$

The Kadar-Parisi-Zhang equation



- Growth is lateral, up to second order

$$\dot{h}(\mathbf{x}, t) = f\left[(\nabla h(\mathbf{x}, t))^2, \Delta h(\mathbf{x}, t), \eta(\mathbf{x}, t)\right]$$

The Kadar-Parisi-Zhang equation

$$\dot{h}(\mathbf{x}, t) = \nu \Delta h(\mathbf{x}, t) + \lambda (\nabla h(\mathbf{x}, t))^2 + \eta(\mathbf{x}, t)$$

- Nonlinear
- Stochastic
- Partial differential equation

Discretization in 1D of the KPZ-equation

Space discretization (1+1 dimensions):

$$x_i = i\Delta x,\ h_i = h(x_i)$$

$$\frac{\partial h}{\partial x}(x_i) = \frac{h_{i+1} - h_{i-1}}{2\Delta x} + O\left(\Delta x^2\right)$$

$$\left[\frac{\partial h}{\partial x}(x_i)\right]^2 = \frac{\left(h_{i+1} - h_{i-1}\right)^2}{4\Delta x^2} + O\left(\Delta x^2\right)$$

$$\frac{\partial^2 h}{\partial x^2}(x_i) = \frac{h_{i+1} - 2h_i + h_{i-1}}{\Delta x^2} + O\left(\Delta x^2\right)$$

$\Downarrow$

$$\frac{\mathrm{d}h_i}{\mathrm{d}t} = \frac{1}{\Delta x^2}\left[\nu\left(h_{i+1} - 2h_i + h_{i-1}\right) + \frac{\lambda}{4}\left(h_{i+1} - h_{i-1}\right)^2\right] + \text{noise.}$$

Numerical solution of the KPZ-equation

- ξ is a random number with zero mean (can be Gaussian, or uniform)
- Due to noise Euler scheme is enough:

$$h_i(t+\Delta t) = h_i(t) + \nu \frac{\Delta t}{(\Delta x)^2}\left[h_{i+1}(t) - 2h_i(t) + h_{i-1}(t)\right] + \\ + \frac{\lambda}{4}\left[h_{i+1}(t) - h_{i-1}(t)\right] + \xi_i$$

- Critical exponents and and universality classes $\alpha = 1/2$, $z = 3/2$

Subjects

- Self-Organized Criticality
  - Bak-Tang-Wiesenfeld model
  - Forest fire model
  - Bak-Sneppen model of evolution
- Traffic models
- 1d driven systems

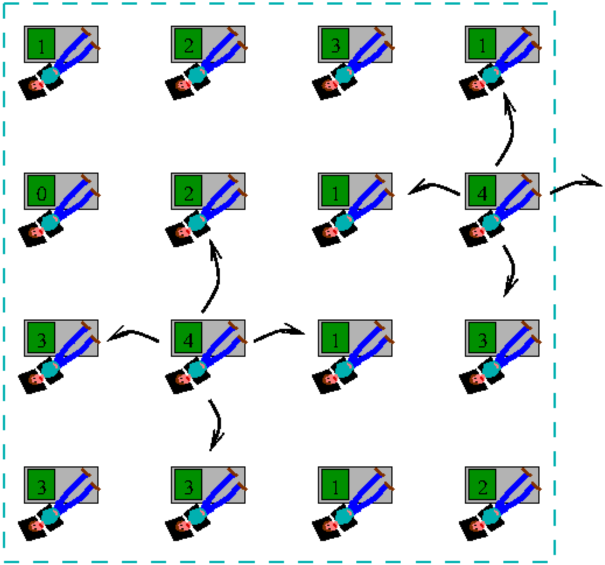
Self-Organized Criticality

- Critical state: inflection point in the critical isotherm
- Power law functions of correlation length, relaxation time
- Control parameter, generally temperature
- Critical point as an attractor?
- Why? Power law: We see many cases
  - $1/f$ noise (music, ocean, earthquakes, flames)
  - Lack of scales (market, earthquakes)
- Underlying mechanism?

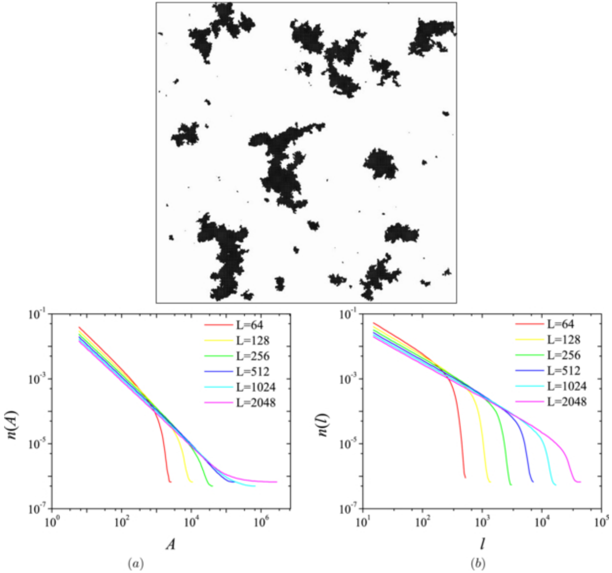
Bak-Tang-Wiesenfeld model

- Originally a sandpile model
- Better explained as a *Lazy Bureaucrat model*:
  - Bureaucrats are sitting in a large office in a square lattice arrangement
  - Occasionally the boss comes with a dossier and places it on a random table
  - The bureaucrats do *nothing* until they have less than 4 dossiers on their table
  - Once a bureaucrat has 4 or more dossiers on its table starts to panic and distributes its dossiers to its 4 neighbors
  - The ones sitting at the windows give also 1 dossier to its neighbors and throw the rest out of the window.

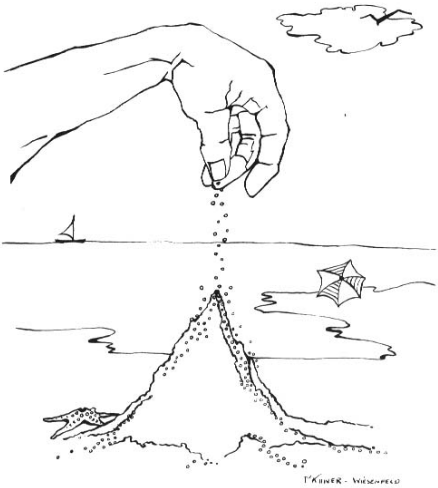
Bak-Tang-Wiesenfeld model



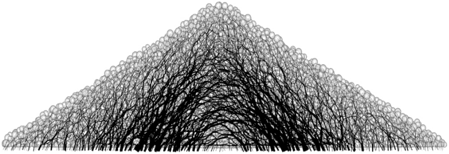
Bak-Tang-Wiesenfeld results



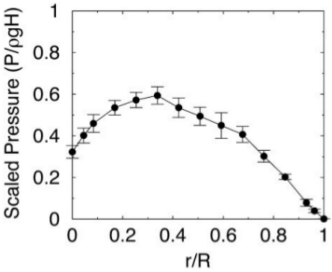
Sandpile experiment

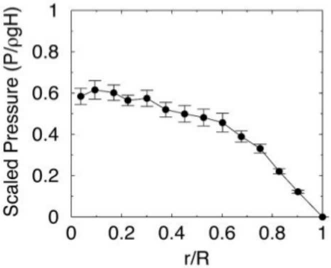


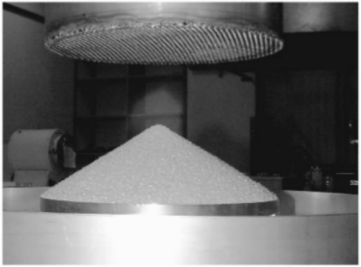
Dip under the heap



Dip under the heap







Forest fire

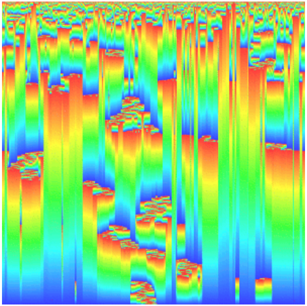
Forest fire model

- Burning cell turns into an empty cell
- A tree will burn if at least one neighbor is burning
- A tree ignites with probability f even if no neighbor is burning
- An empty space fills with a tree with probability p

- Control parameter p/f the average number of trees planted between two lightning strikes
- Histogram of burned forest size is a power law

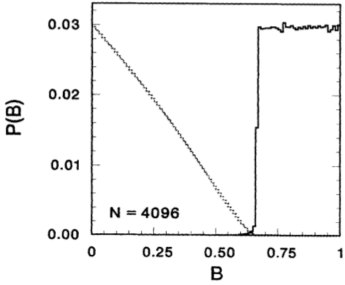
Bak-Sneppen model of evolution

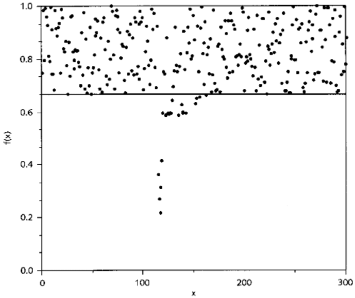
- N species all depends on two other (ring geometry)
- Each species are characterized by a single *fitness*
- In each turn the species with the lowest fitness dies out and with it its two neighbors irrespective of their fitness
- These 3 species are replaced by new ones with random fitness
- Inital and update fitness is uniform between $[0, 1]$

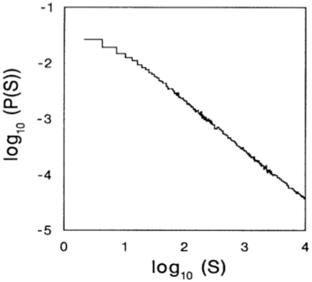


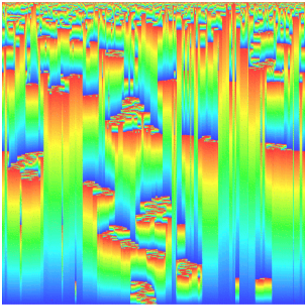
Bak-Sneppen model of evolution: Results

- Steady state with avalanches
- Avalanches start with a fitness $f > f_c \simeq 0.66$
- Avalanche size distribution power law
- Distance correlation power law

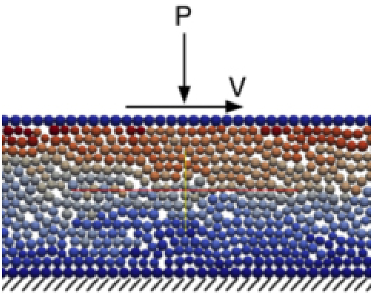

P(B)
0.03
0.02
0.01
0.00
N = 4096
0
0.25
0.50
0.75
1
B

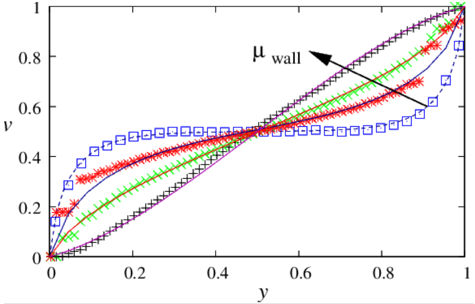

f(x)
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
x

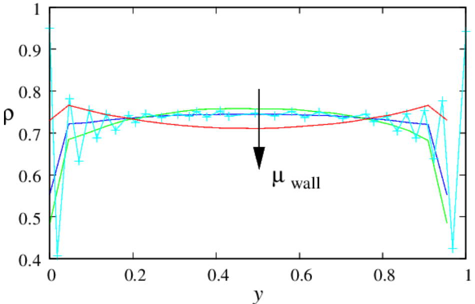

$\log_{10}$ (P(S))
-1
-2
-3
-4
-5
0
1
2
3
4
$\log_{10}$ (S)



Bak-Sneppen model of evolution an application: Granular shear





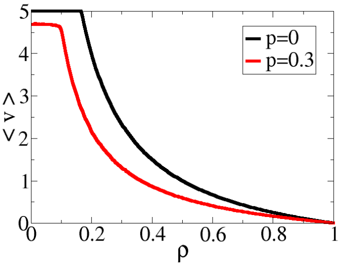


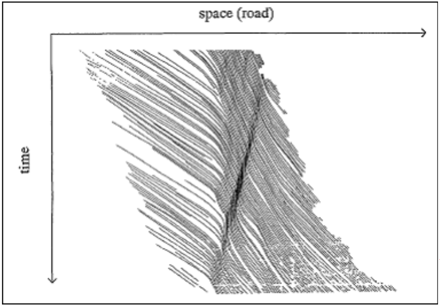
Traffic models

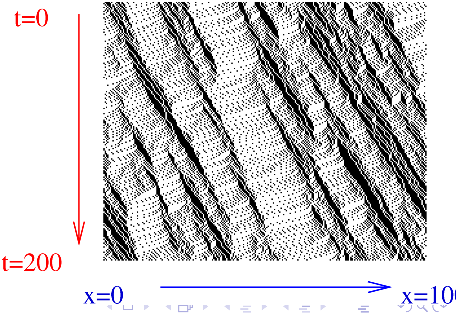
Nagel–Schreckenberg model

- Periodic 1d lattice (ring) Autobahn
- Cars occupying a lattice moving with velocities $0, 1, 2, 3, 4, 5$
- Remark, if max speed is 126 km/h, then lattice length is 7 m, a very good guess for a car in a traffic jam
- It uses parallel update
- Simultaneously each car adjusts its speed according to rules:
  1. **Acceleration**: All cars not at the maximum velocity increase their velocity by 1
  2. **Slowing down**: Speed is reduced to distance ahead (1 sec rule)
  3. **Randomization**: With probability p speed is reduced by 1
  4. **Car motion**: Each car moves forward the number of cells equal to their velocity.

Emergence of traffic jams





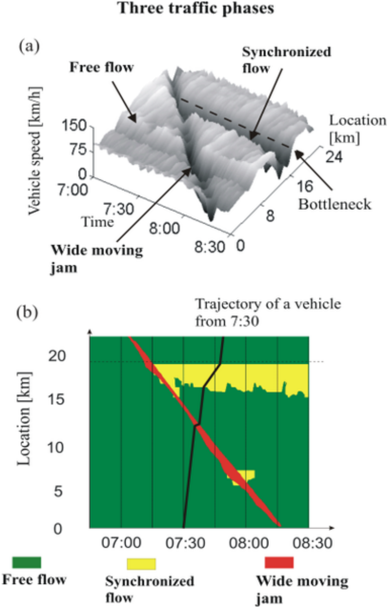


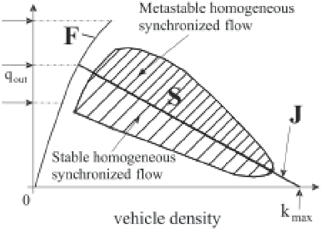
Nagel–Schreckenberg model

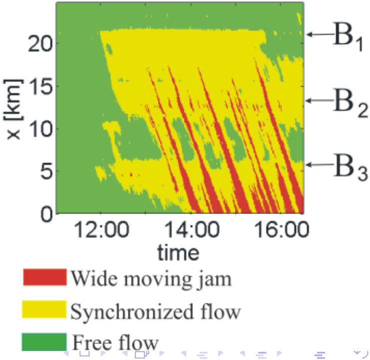
- Transition from free-flow to jammed state
- Jammed state is a phase-separated phase
- Without randomization a sharp transition
- Used in NRW to predict traffic jams

autobahn.NRW
Hochrechnung für Bundesautobahnen
Montag, 01.07.2013, 08:05 h
aktuelle Verkehrslage
Prognose 30 min
Prognose 60 min
Langzeit Prognose
Fahrzeitprognose
Farbmodus: Standard
Baustelleninfo
Verkehrsdichten
frei
zähfließend
dicht
gestaut
Baustelle mit geringer Staugefahr
Baustelle mit hoher Staugefahr
Anschlussstelle
Sperrung der Autobahn
Vollsperrung der Anschlussstelle
Teilsperrung der Anschlussstelle
Informationen
Impressum
Version 3.6.1
0 km
15 km
Wesel
Recklinghausen
Lünen
Gelsenk.
Bottrop
Herne
Dortmund
Kamp-Lintfort
Oberhsn.
Essen
Moers
Bochum
Duisburg
Mülheim
Witten
Kempen
Krefeld
Hagen
Velbert
Viersen
Gevelsberg
Düsseldorf
Mönchengladbach
Neuss
Wuppertal
Lüdenscheid

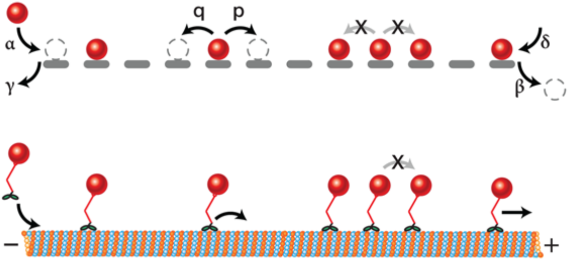
Three-phase traffic theory





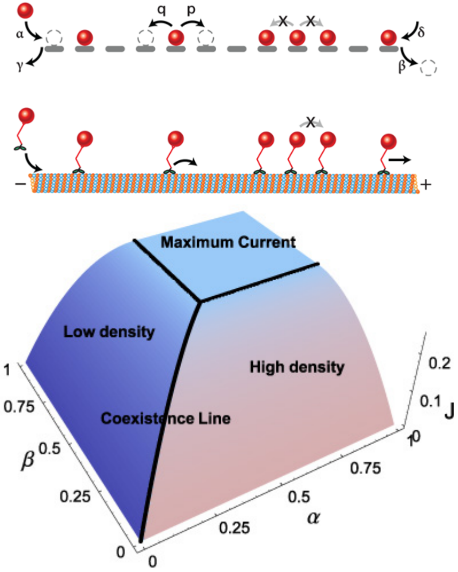


Asymmetric simple exclusion process



- $p + q = 1$
- If $p = q$ then SEP a Markov-process
- Generally $\gamma = \delta = 0$
- α and β determines the phase diagram

Asymmetric simple exclusion process



Three state ASEP

$$+\ 0 \xrightarrow{\alpha} 0\ + \quad ; \quad 0\ - \xrightarrow{\alpha} -\ 0 \quad ; \quad +\ - \underset{q}{\overset{1}{\rightleftarrows}} -\ +$$

- If q small three blocks $(00\dots00++\cdots++--\cdots--)$
- Mixed state above $q = 1$
- Numerical simulations suggested an other phase transition at $q_c < 1$
- Actually false, only correlation length is finite but large $\sim \mathcal{O}(10^{70})$
- Correspondence to Zero Range Process