

Computer Simulations in Physics

Course for MSc physics students

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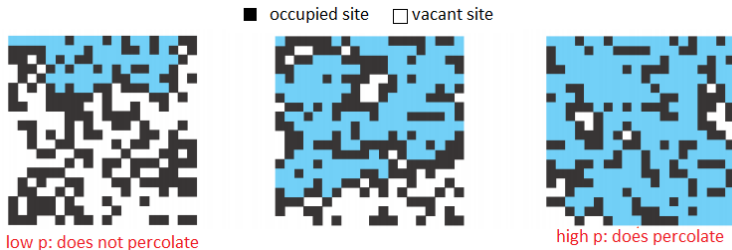
March 2, 2021

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 law away from the critical density
4. Power law

Percolation theory

Questions (in infinite systems):

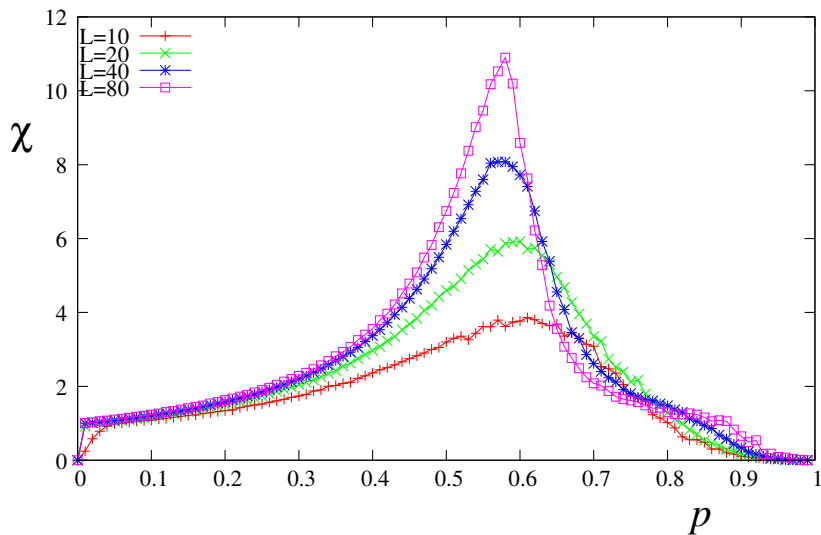
1. Is there an infinite cluster in infinite systems?
2. How many infinite clusters are there?
3. Cluster size distribution (n_s)
4. Mean cluster size (without the infinite one)? ($S = \sum_s s^2 n_s$)

Answers:

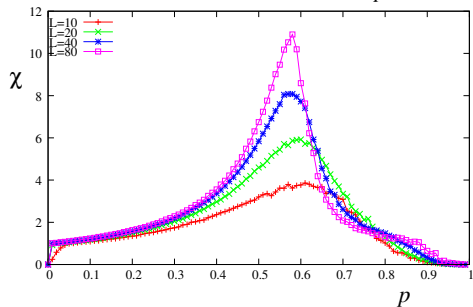
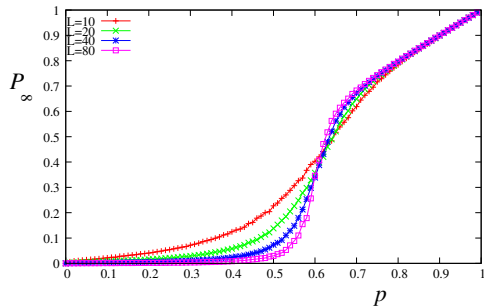
1. if $p > p_c$ then yes, otherwise no
2. Only 1!
3. $n_s \sim s^{-\tau}$
4. $S \sim |p - p_c|^{-\gamma}$

Like a second order phase transition in a geometric system!

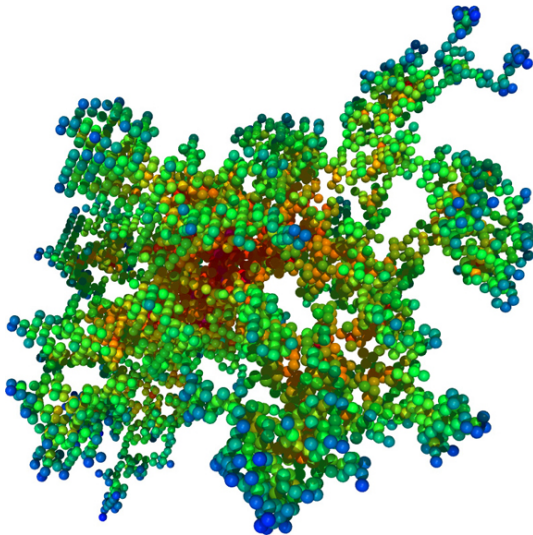
Percolation model



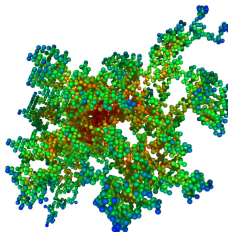
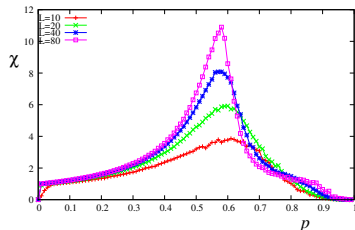
Percolation model



Percolation model



Percolating cluster



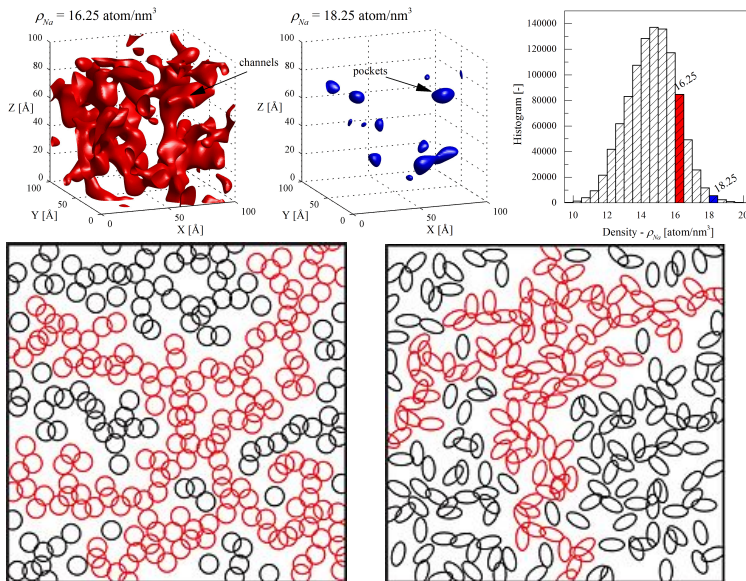
► Largest cluster

- fractal with fractal dimension of d_f

$$\text{► } S_\infty \sim \begin{cases} \xi_f^d \log(N/\xi_f^d) & p < p_c \\ N^{d_f/d} & p = p_c \\ NP_\infty(p) & p > p_c \end{cases}$$

- 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
- ▶ Flodings



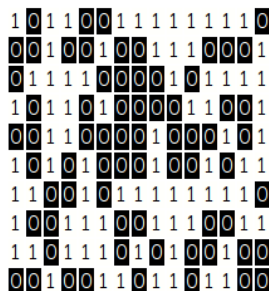
Percolation model

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]

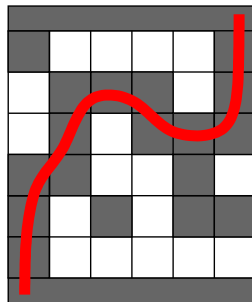
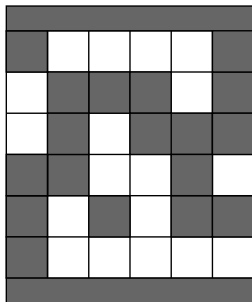
Hoshen-Kopelman Algorithm

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

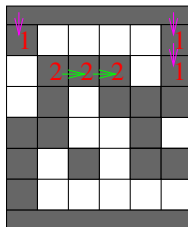
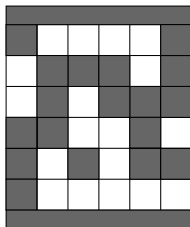


Hoshen-Kopelman Algorithm

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



Hoshen-Kopelman Algorithm

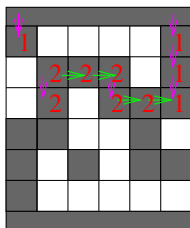


link[1]=1

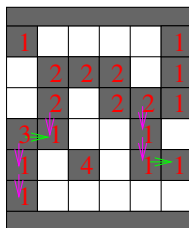
link[2]=2

- ▶ 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



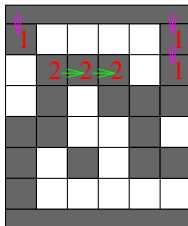
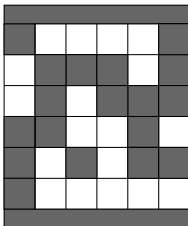
```
link[1]=1
link[2]=1
```



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

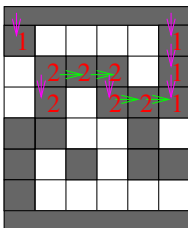
- ▶ ...
- ▶ If site is occupied, look left and up
 - ▶ ...
 - ▶ if both sites are occupied \rightarrow then link the two
 - ▶ a link which points to itself is a root link
 - ▶ find the root of both sites
 - ▶ connect the larger to the smaller
 - ▶ use this number

Hoshen-Kopelman Algorithm



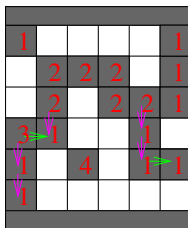
link[1]=1

link[2]=2



link[1]=1

link[2]=1



link[1]=1

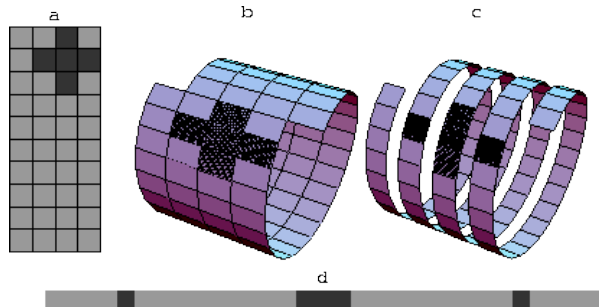
link[2]=1

link[3]=1

link[4]=4

Hoshen-Kopelman Algorithm

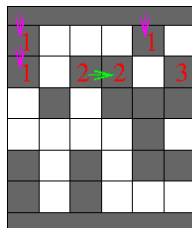
- ▶ Site percolation
- ▶ Helical boundary conditions (rolled up onto 2D lattice)
- ▶ Go through site in typewriter style
- ▶ Check left and above (as before)



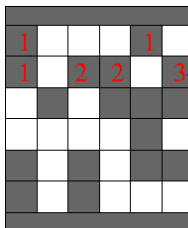
Hoshen-Kopelman Algorithm

- ▶ 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

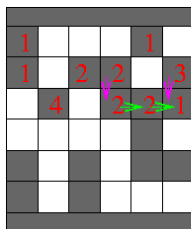
Hoshen-Kopelman Algorithm, Periodic BC



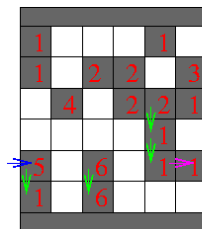
link[1]=1
link[2]=2
link[3]=3



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

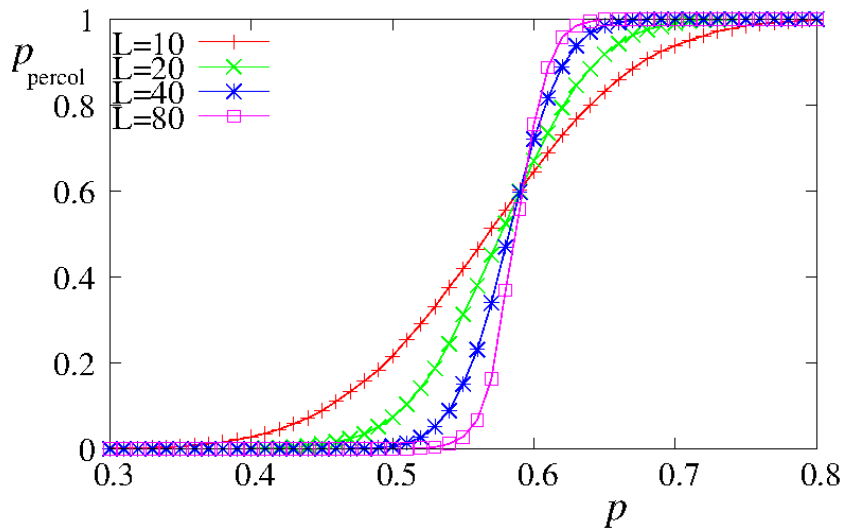


link[1]=1
link[2]=1
link[3]=1
link[4]=4



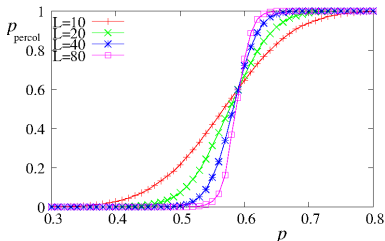
link[1]=1
link[2]=1
link[3]=1
link[4]=4
link[5]=1
link[6]=6

Result

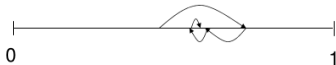


Determine p_c

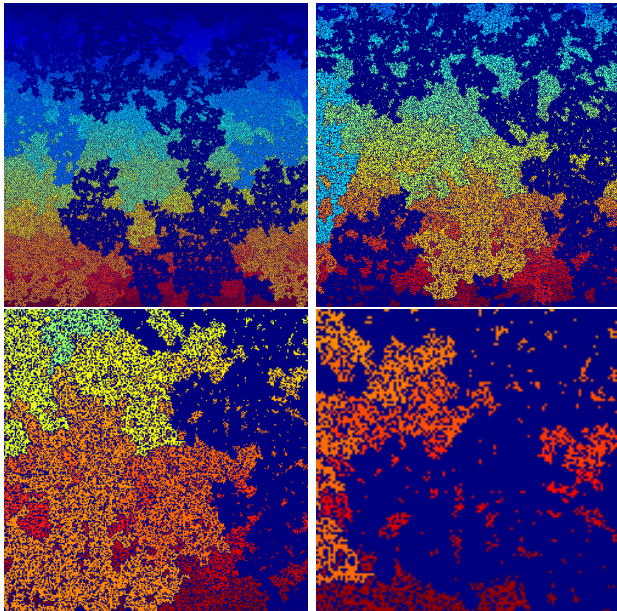
- From order parameter:



- Increase and decrease p by $p/2$ to converge to p_c
- Use the monotonicity of the percolation
- Same random number sequence can be generated!



Self similarity



Fractals



Mandelbrot set:

$f_c(z) = z^2 + c$, $z, c \in \mathbb{C}$ for which $f_c(0)$, $f_c(f_c(0))$ remains bounded in absolute value.



Fractal growth

Fractal growth



Electrochem. deposition



Mineralization

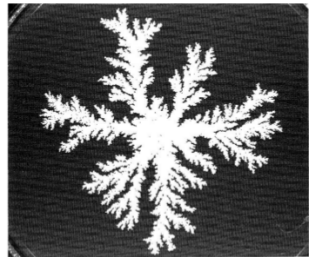


Surface crystallization



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

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

- ▶ Boundary condition: potential is curvature (κ) dependent

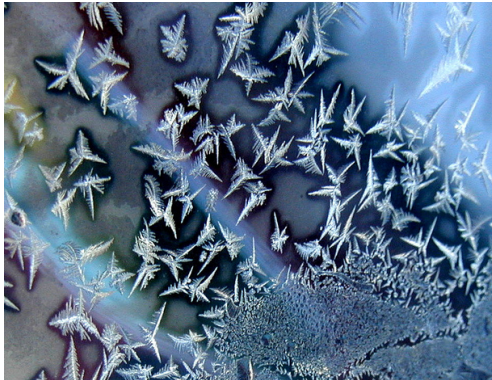
$$u|_{\Gamma} = f(\nabla u, \kappa)$$

- ▶ Disorder: small fluctuations

Fractal growth

Laplacian or gradient governed growth

- ▶ Scalar field (electrostatic field, density, through diffusion)
- ▶ Velocity of the interface Γ proportional with the gradient
- ▶ Boundary condition: potential is curvature (κ) dependent
- ▶ Disorder: small fluctuations



Fractal growth

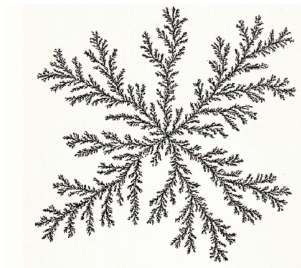
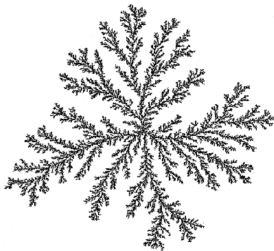
Consequences:

- ▶ *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

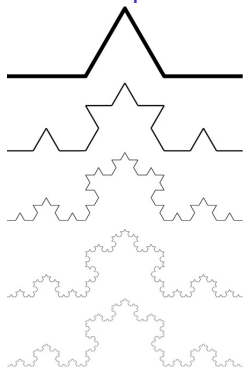
- ▶ Self-similarity
- ▶ Repeating pattern
- ▶ Scaling patterns



Scale invariance



Fractal dimension: Example



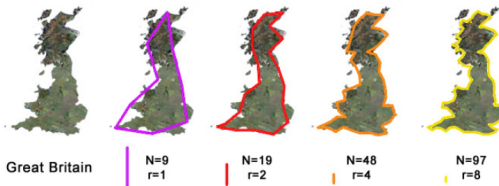
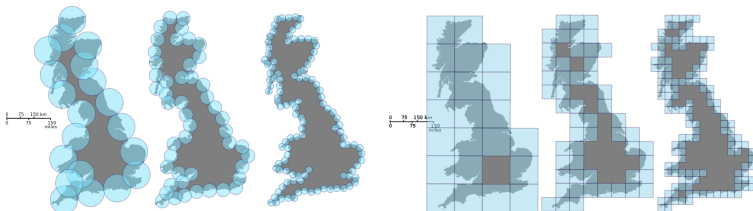
Koch curve

- ▶ 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:

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

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:

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

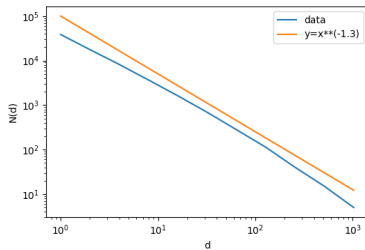
- ▶ Differences:

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

- ▶ In practice

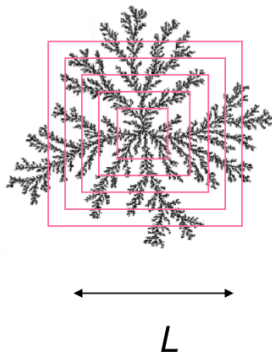
$$N(\varepsilon) \propto \varepsilon^D$$

Fractal dimension



Fractal dimension: Other methods

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



- Correlation functions

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

$$D = d - \alpha$$

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:

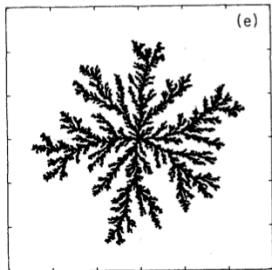
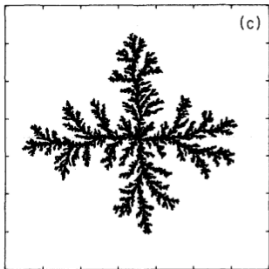
- ▶ Start with a seed at $(0,0)$
- ▶ Start random walker on a circle just big enough to cover the cluster
- ▶ Define a kill ring big enough or use reentry distribution
- ▶ Regions of large jumps, on a larger scale lattice



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).

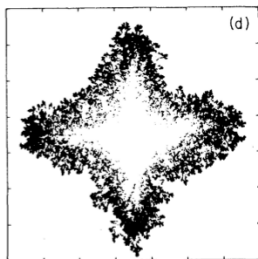
DLA: Lattice effects

10^6 particles

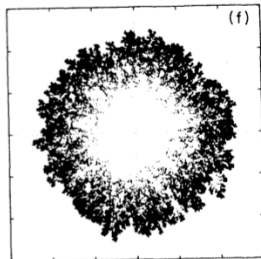


10 clusters of 10^5 particles

on-lattice

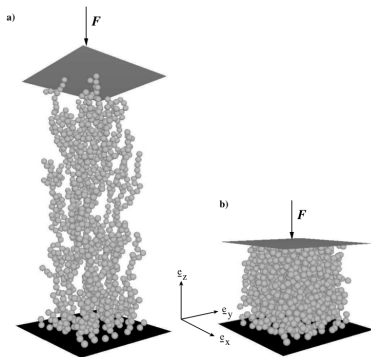
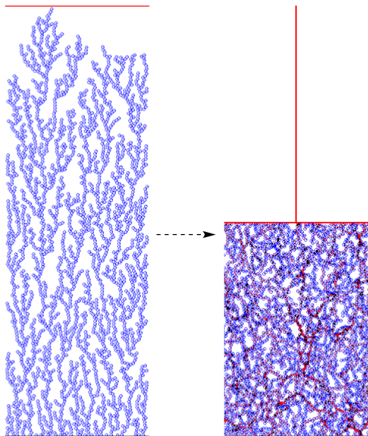
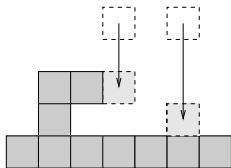


off-lattice



Ballistic deposition

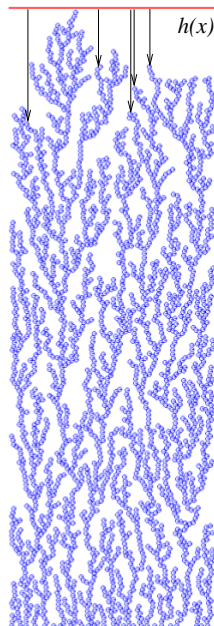
- ▶ Lattice
- ▶ Off lattice



Surface growth models

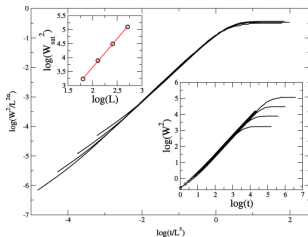
- ▶ Not the whole object but only its surface is interesting (e.g. coastline)
- ▶ Object starts from a d -dimensional substrate
- ▶ Object grows in the $d + 1$ th dimension.
- ▶ Object is described by $h(x)$ (x is a d -dimensional position vector) height function which is the maximum surface position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

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



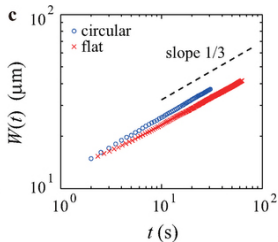
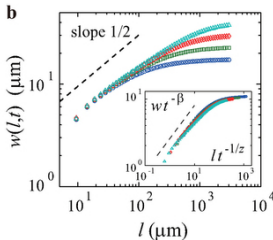
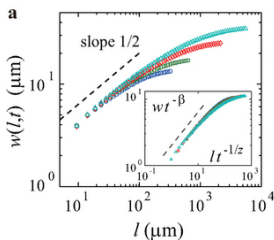
Family-Vicsek scaling

- Change of width in time



- Scaling relation:

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



Theory: The KPZ-equation

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

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

- ▶ Normally:

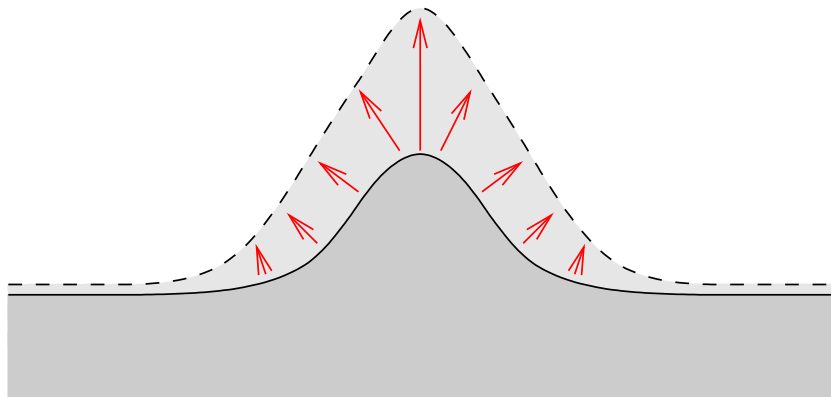
$$\dot{h}(x, t) = f[h(x, t), \nabla h(x, t), \Delta h(x, t), \eta(x, t)]$$

- ▶ Gaussian noise:

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

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

The Kadar-Parisi-Zhang equation



- Growth is lateral, up to second order

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

The Kardar-Parisi-Zhang equation

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

- ▶ Nonlinear
- ▶ Stochastic
- ▶ Partial differential equation

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:

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

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

Practice: Hoshen-Kopelman Algorithm

- ▶ Fill a square lattice with random 0 and 1
- ▶ Create a large enough array where `link[i]=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.