Simulations in Statistical Physics

Course for MSc physics students

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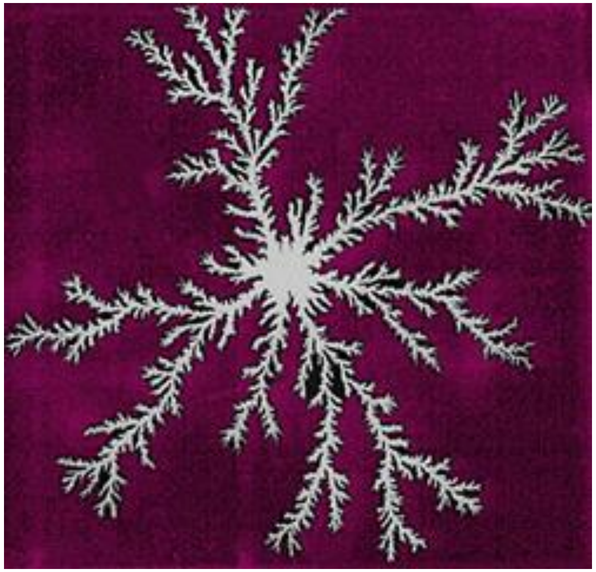
Algorithmically defined models

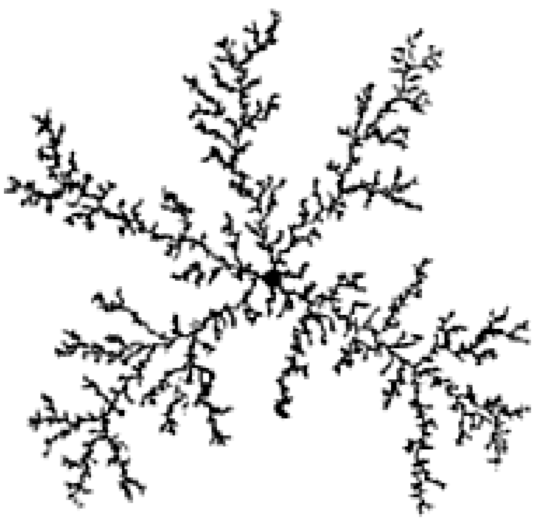
Fractal growth



Elctrochem. deposition

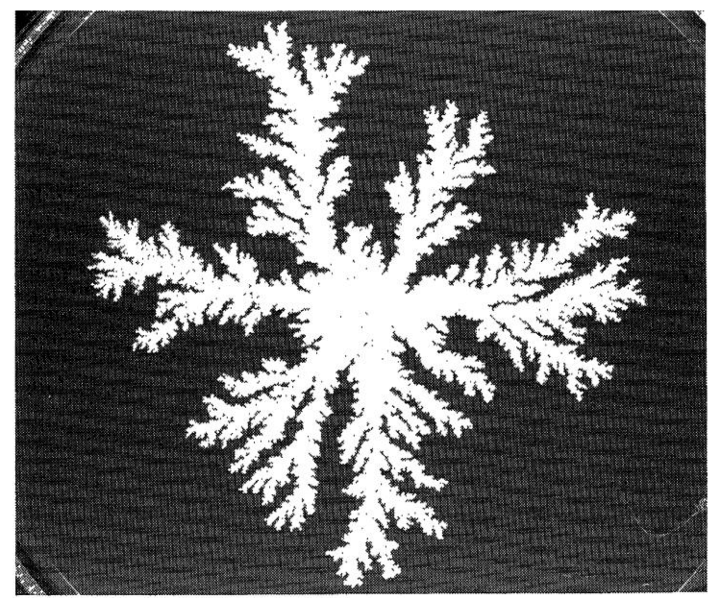
Mineralization

Surface crystallization



Disordered viscous fingering

Bacterial colony growth



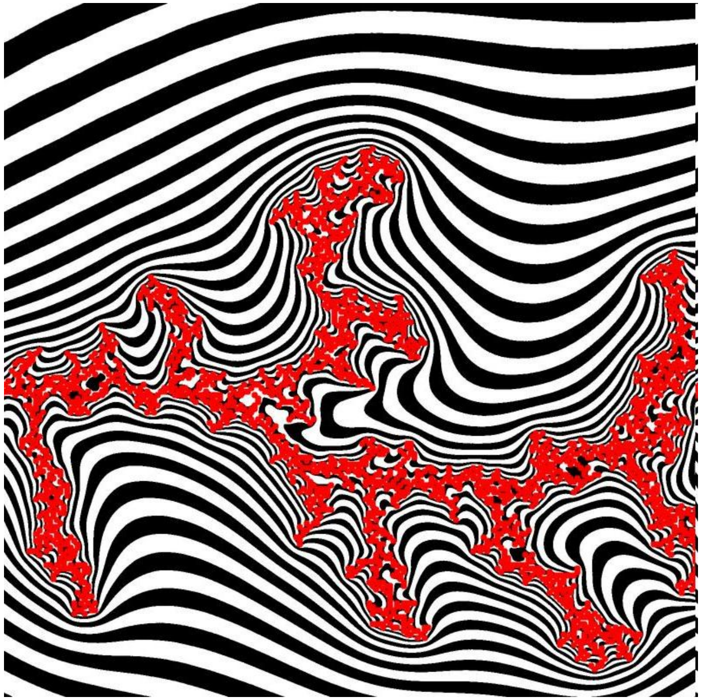
Basic equations:

$$\nabla^2 u = 0 \qquad u \text{ scalar field } (T, P, c\ldots)$$

$$\mathbf{v}\big|_\Gamma = -C\nabla u\big|_\Gamma \qquad \mathbf{v} \text{ velocity of the interface } \Gamma$$

$$u\big|_\Gamma = f(\nabla u, \kappa) \qquad \kappa \text{ curvature (cutoff)}$$

$$+ \text{ disorder}$$



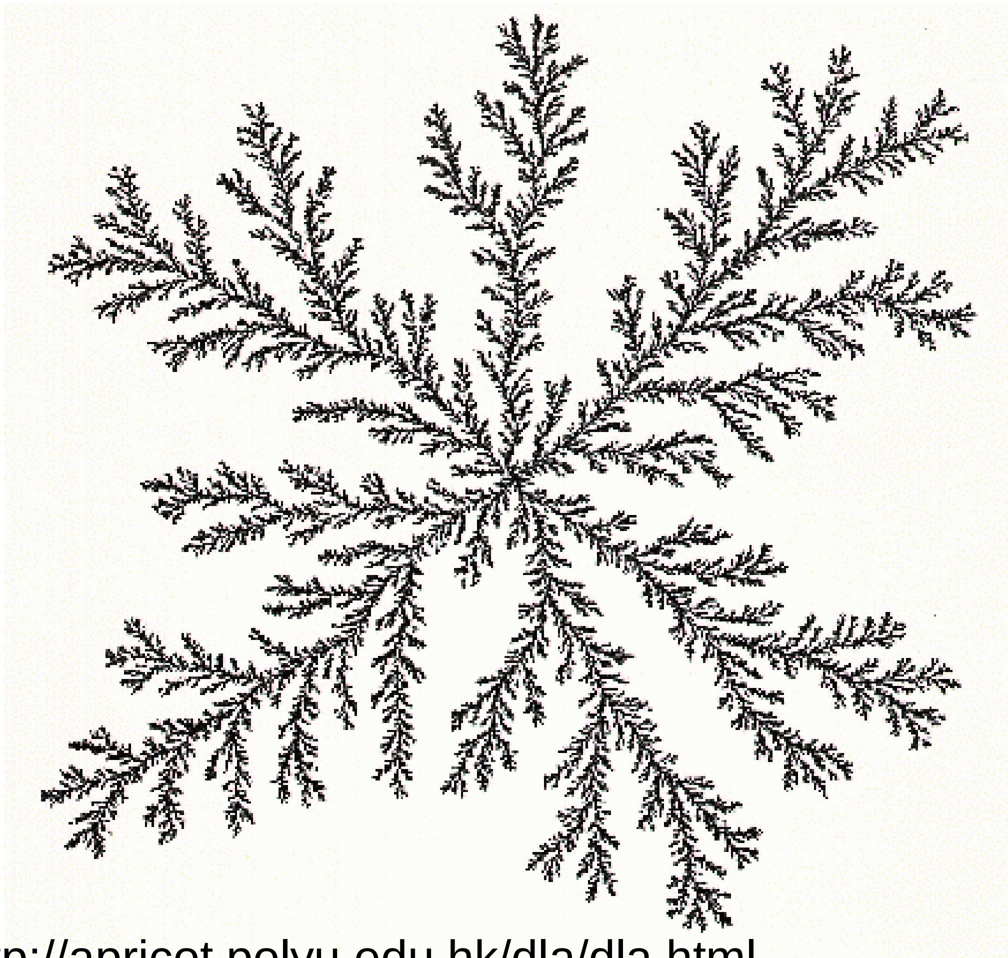
Laplacian or gradient governed groth:

If there is a bump, the gradient increases (c.f. electrostatic peak effect) the bump grows… instability

+ screening:
If 2 bumps grow, the faster will screen the slower and stop its growth

Simple model: Diffusion limited aggregation (DLA)

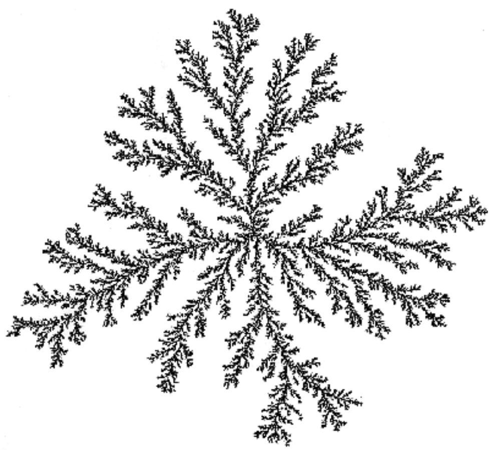
Start with a seed particle forming the initial aggregate.
* Another particle comes from infinity via a random walk until it sticks to the aggregate.
Goto *



100 million particles

Coarsened

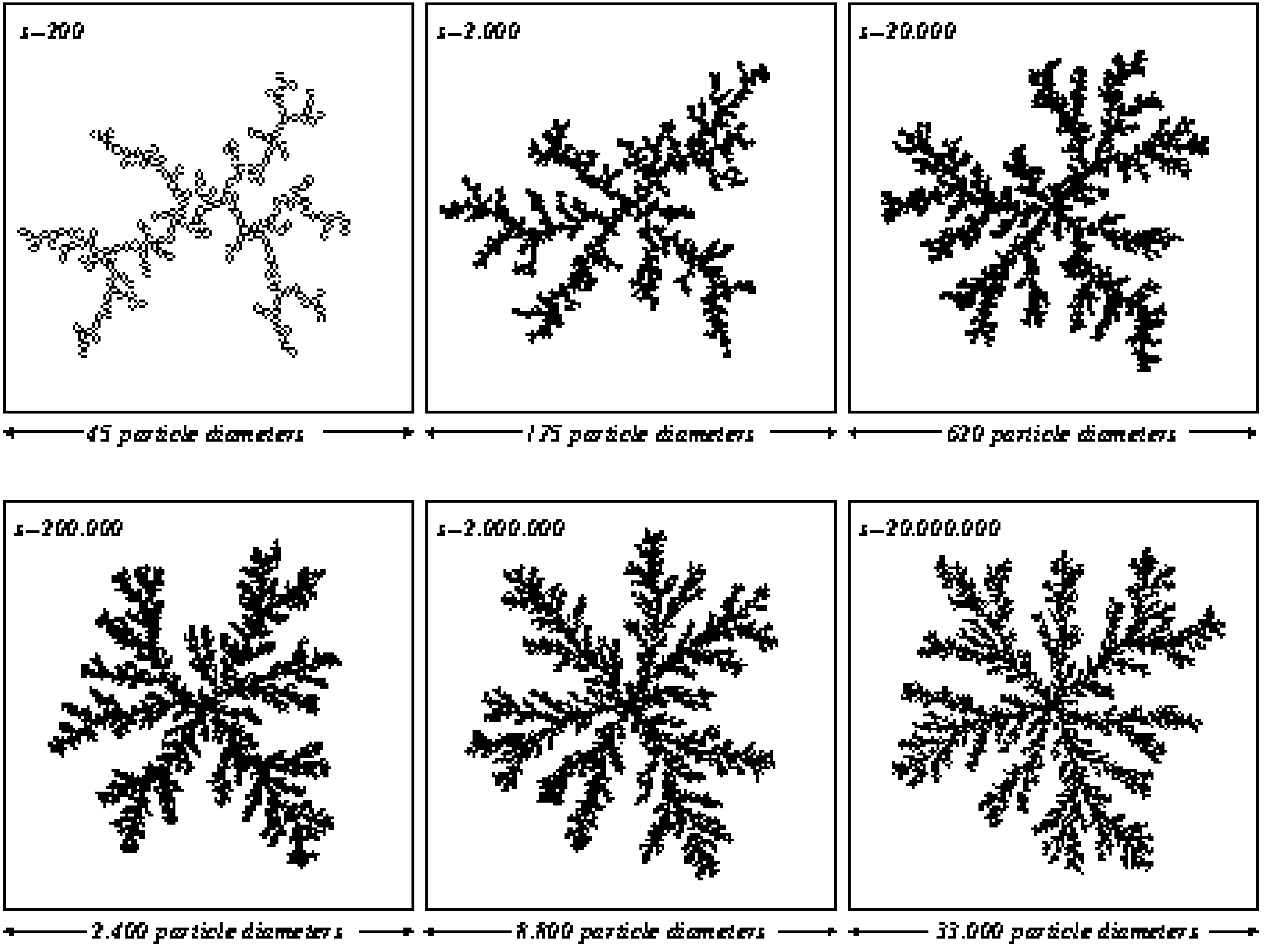
Self-similar structure



1 million particles

http://apricot.polyu.edu.hk/dla/dla.html

Illustration of statistical self-similarity



In order to simulate (relatively) large samples tricks are needed
- Birth ring sorrounding the aggregate
- No need to let the particles walk far away: killing ring
- If far from the aggregate: large steps possible

For very large (>10^7) particles more tricks (fitted step size, dynamic storage)

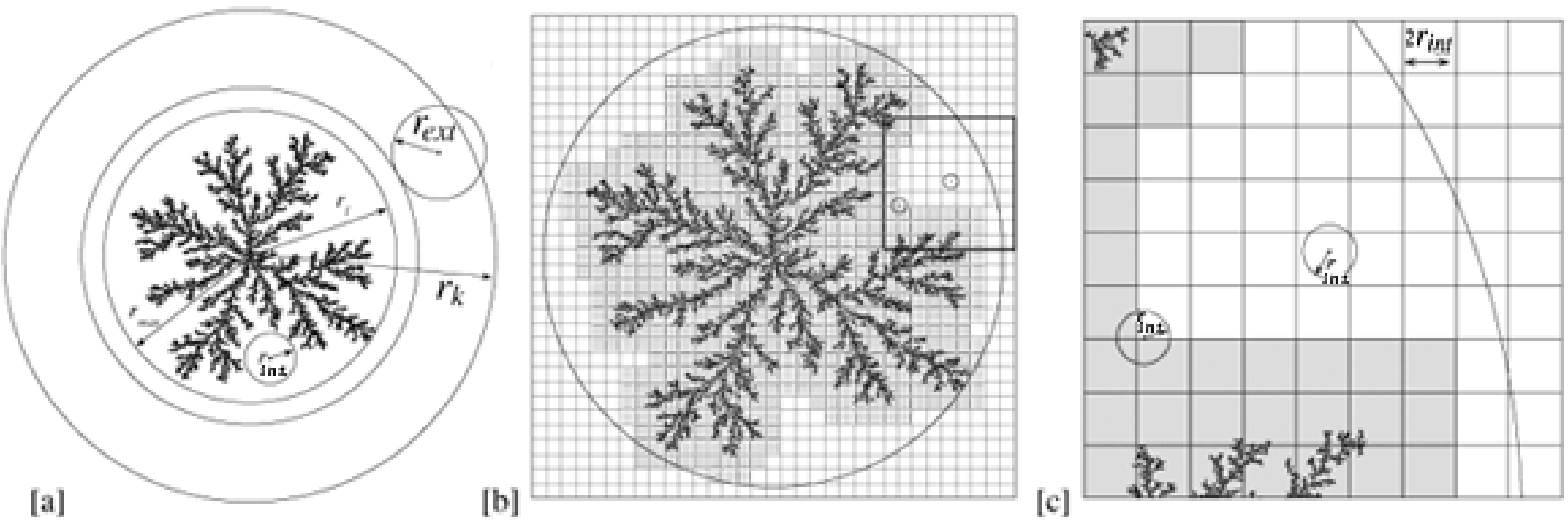


FIG. 1: (a) Schematic representation of the "optimized random trajectories". (b) A DLA aggregate and a mesh of cells $2r_{int} \times 2r_{int}$. Long steps are forbidden in the gray boxes and allowed in the white ones. Also, two long steps are illustrated. (c) A zoom of the region inside the large square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

Why are so terribly large aggregates needed?Self similar fractals, scaling → asymptotic behavior. How to measure fractal dimension?

Dimensions

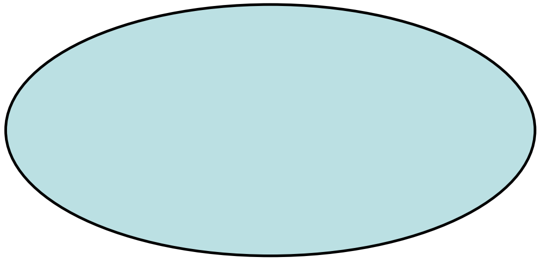
- Topological dimension:

Point: d_t=0, moving point: d_t=1, moving line, d_t=2…

- Embedding dimension:

Number of independent directions

- Hausdorff (fractal) dimension



Area *A* is mesured by covering the object with squares of size ℓ^2. # of such boxes: N_ℓ.

$$A = \lim_{\ell \to 0} \ell^2 N_\ell$$

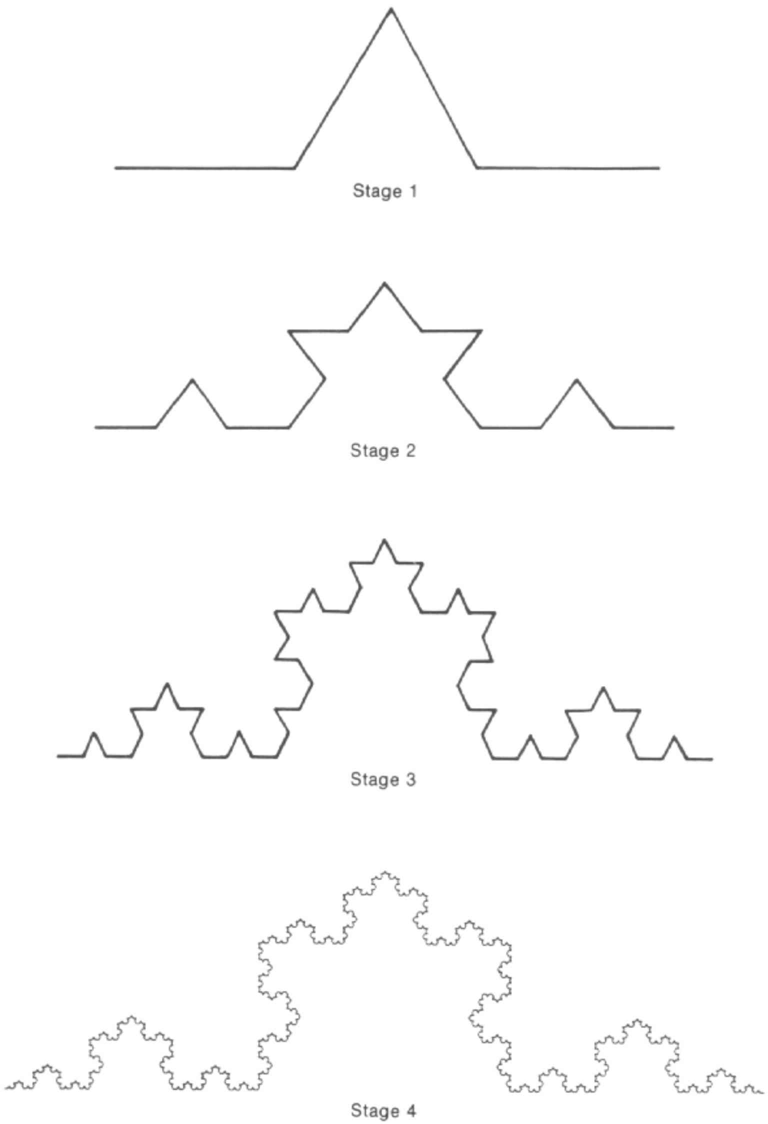
$$L = \lim_{\ell \to 0} \ell^1 N_\ell$$

In general:

$$M = \lim_{\ell \to 0} \ell^{d_t} N_\ell$$

M: mass

For a fractal this definition does not lead to a good result (0 or ∞)



Adapted from Benoit Mandelbrot, *Fractals*.

$$\ell = \left(\frac{1}{3}\right)^n; \quad N_\ell = 4^n; \quad d_t = 1$$

$$M = \lim_{n\to\infty}\left(\frac{4}{3}\right)^n = \infty$$

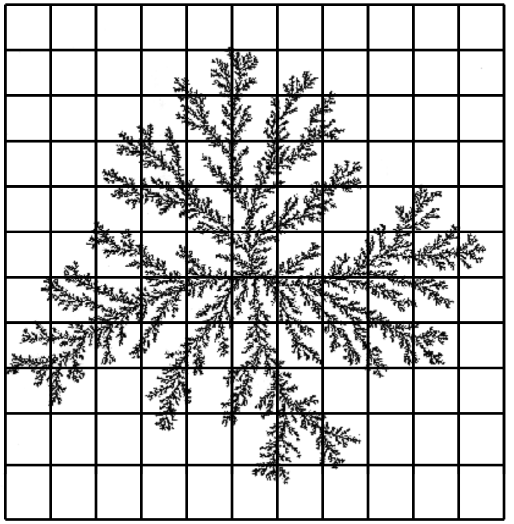
Instead of using d_t find the appropriate D fractal dimension such that

$$M = \lim_{\ell\to 0} \ell^D N_\ell$$ is finite!

Here: $D = \dfrac{\ln 4}{\ln 3}$

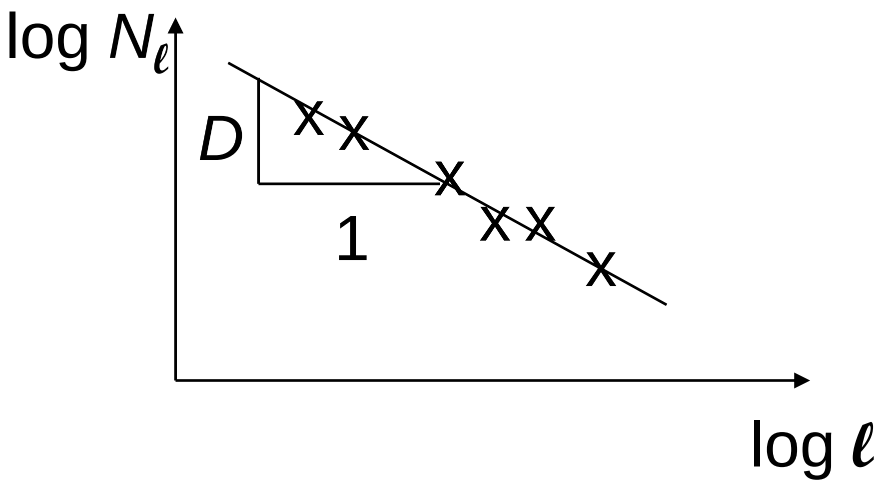
(Def of fractal: $d_t < D < d_e$)

How to measure *D* for a random fractal?

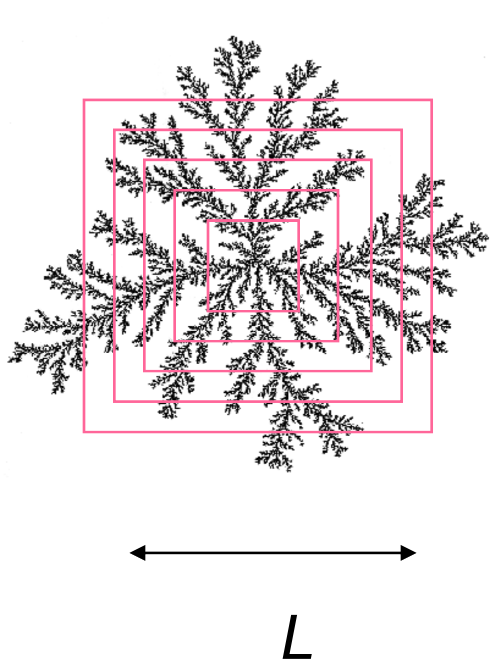


There is always a lower and an upper cutoff (e.g., particle size, radius of gyration).

1. Box counting: Use the definition of *D*. Cover the object with a mesh of mesh size ℓ, count the boxes where there is occupation. Plot log-log the dependence of N_ℓ vs ℓ.



2. Sand box method



$$M \sim L^D$$

3. Correlation functions

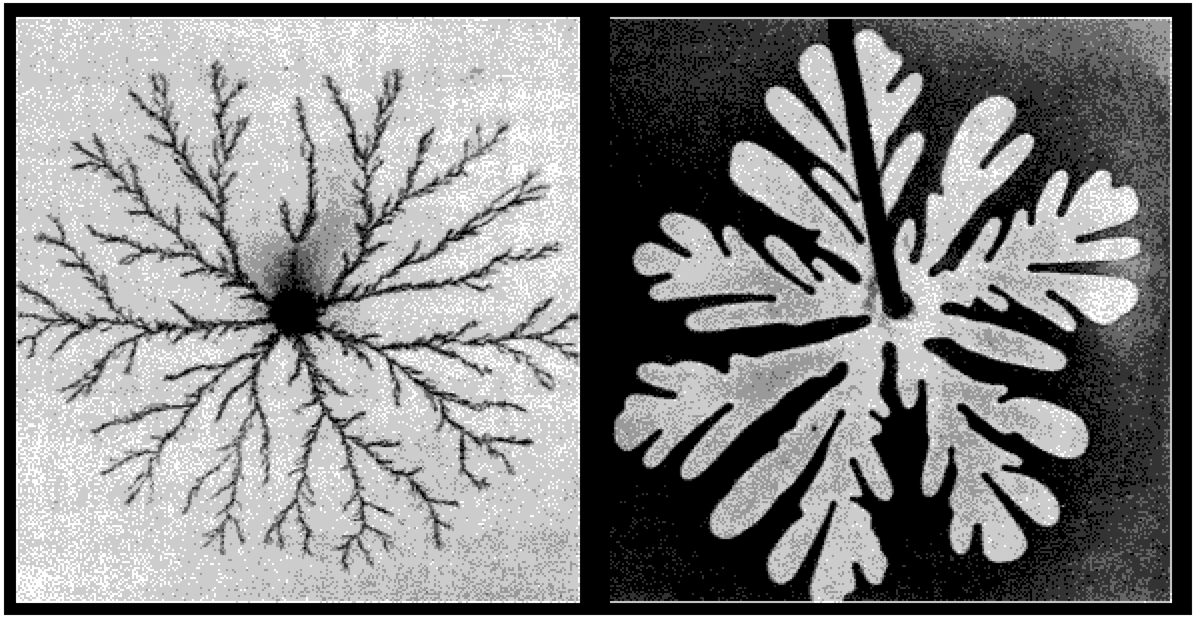
$$C(r) = < \rho(r)\rho(0) > \sim r^{-\alpha}$$

$$\int C(r')d^d r' \sim r^{r-\alpha} \sim M(r)$$

$$D = d - \alpha$$

Lattice effects

Laplacian aggregates have two categories:

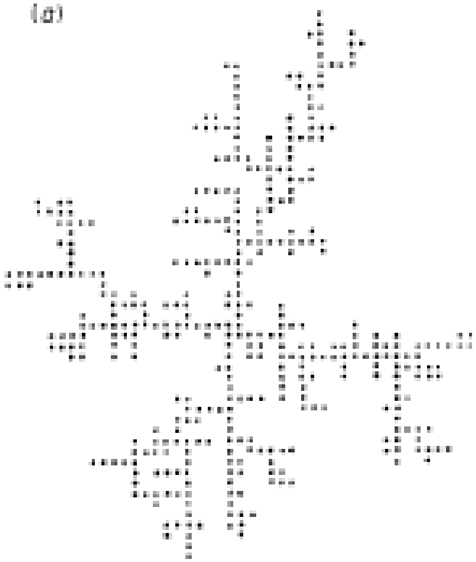


Tip splitting

Stable tips

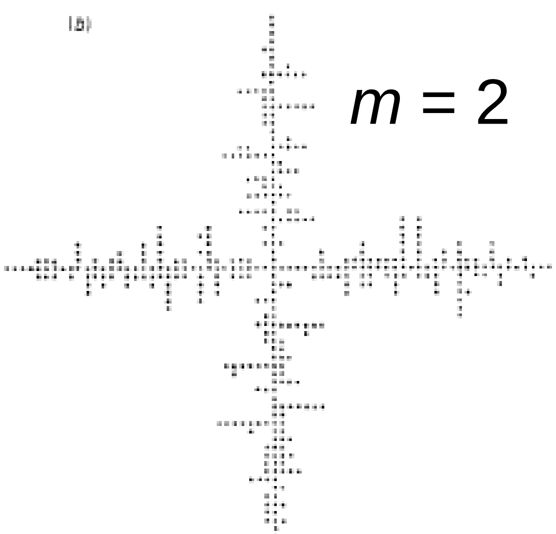
Stabilized by anisotropy

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

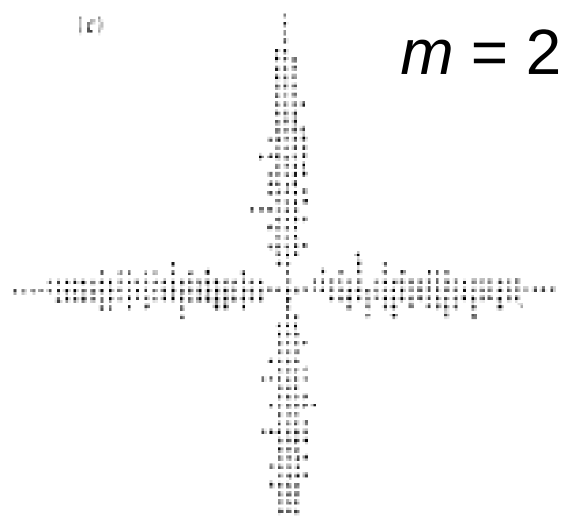


No much difference between lattice and off lattice DLA (a)

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



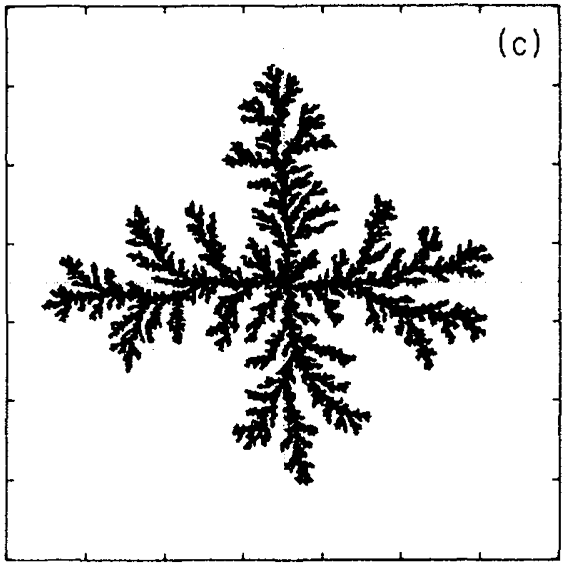
$m = 2$



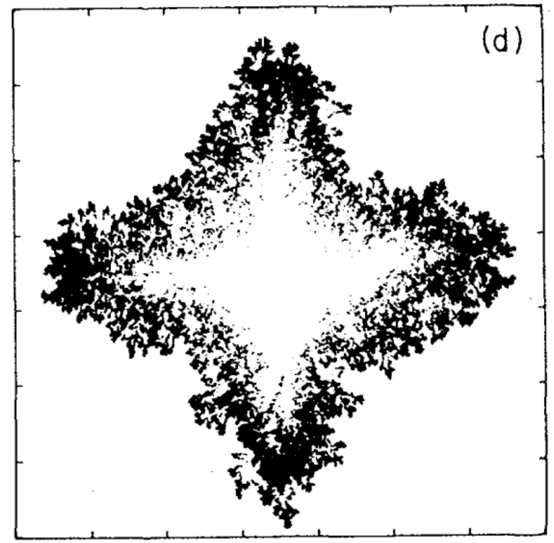
$m = 20$

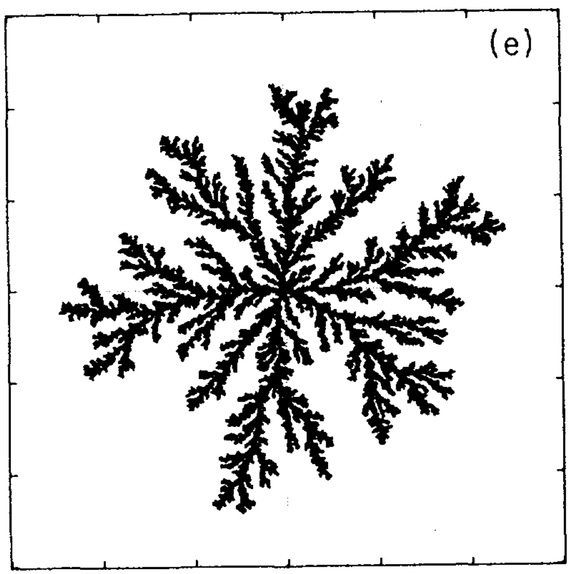
10^6 particles

10 clusters of 10^5 particles

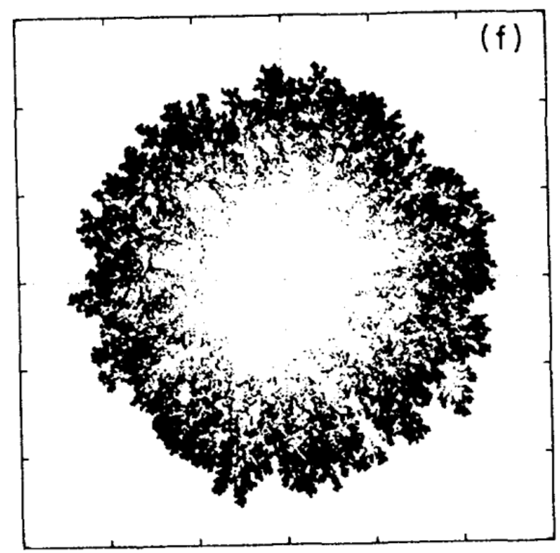


on-lattice





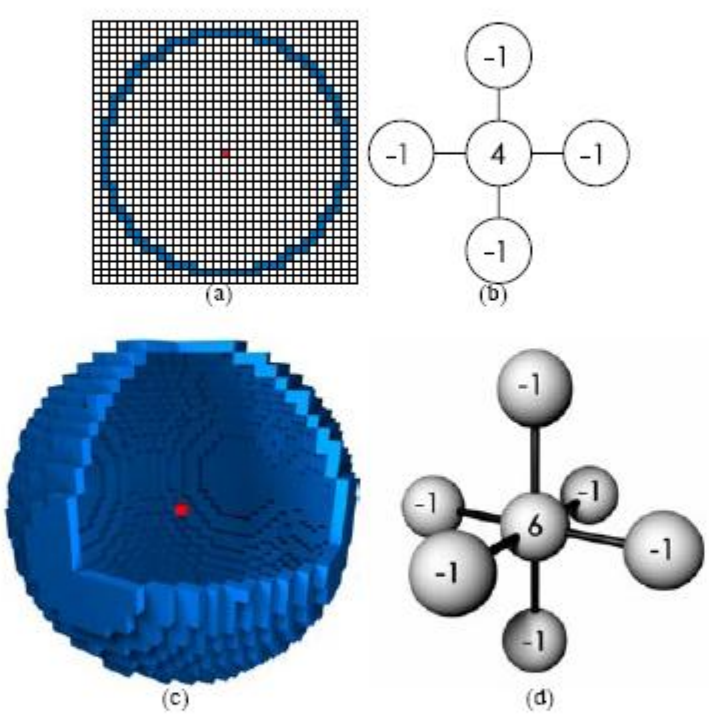
off-lattice



Dielectric breakdown model

We start from a grounded center in 2d (or 3d) sorrounded by a far circle (sphere) held on potential = 1. We solve the Laplace eq. The neighboring sites to the grounded aggregate are growth sites. The growth probability is

$$p_i = \frac{|\nabla u(i)|^{\eta}}{\sum_j |\nabla u(j)|^{\eta}}$$



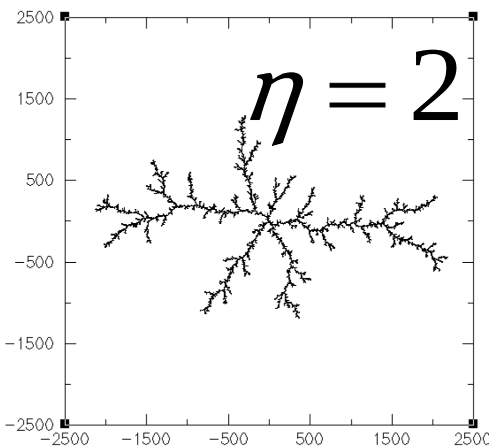
η is a conintuous parameter, which has severe influence on the shape of the aggregates.

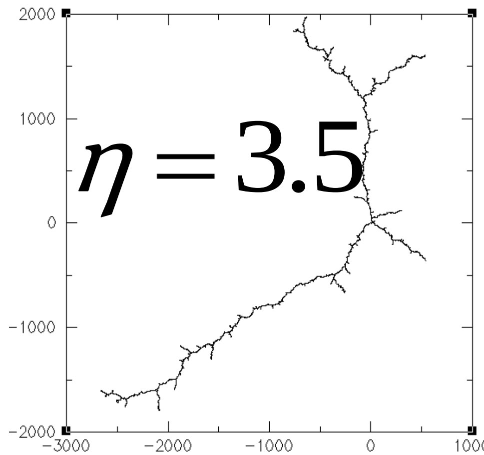
η = 1 corresponds to the DLA case. In fact the patterns are very similar and the fractal dimension too.

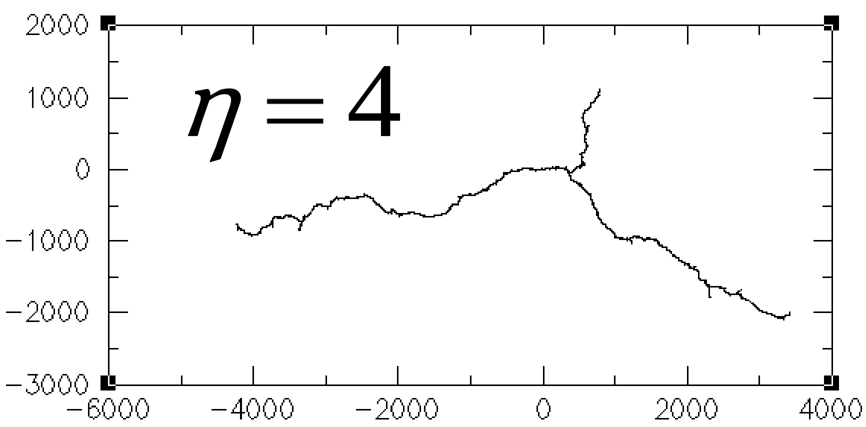
Dielectric breakdown model

←DLA
DBM→

$\eta = 1$







$\eta = 0 \quad D = d$

What is then the role of randomness?

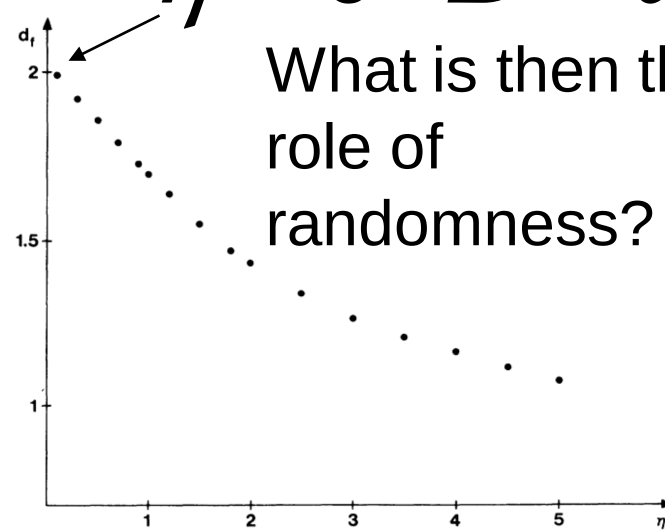


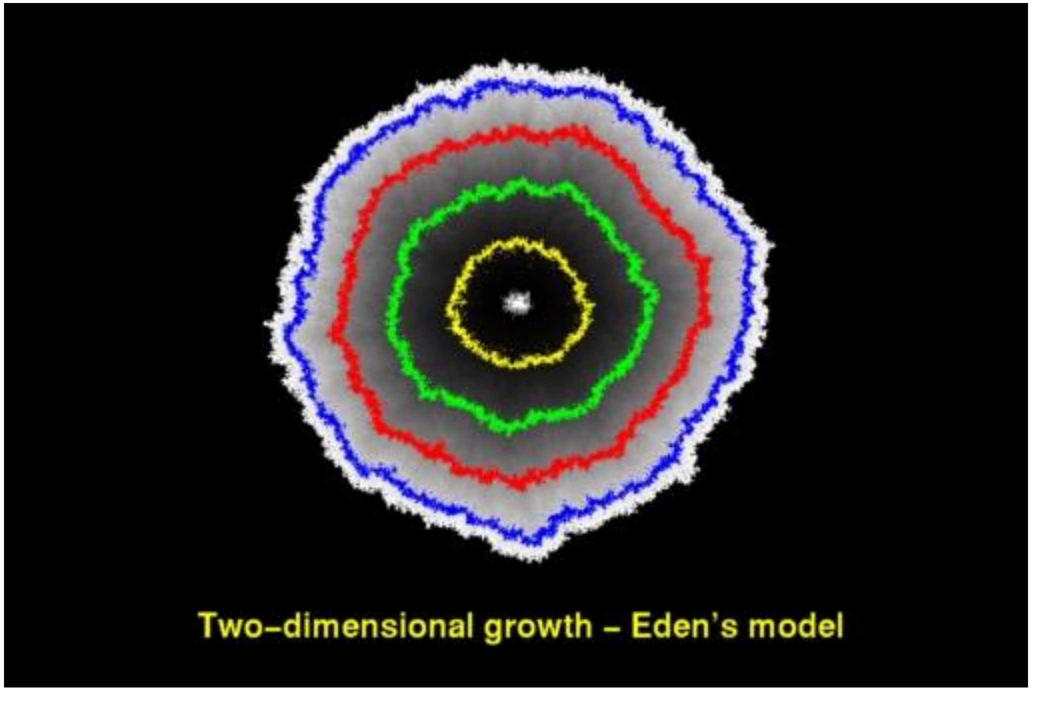
FIG. 1. $d_f(\eta)$.

C. Amitrano: PRA 39 6618 (1989)

The Eden model

If $\eta = 0$ the growth probability becomes independent of the Laplacian field (no need to solve the eq.).

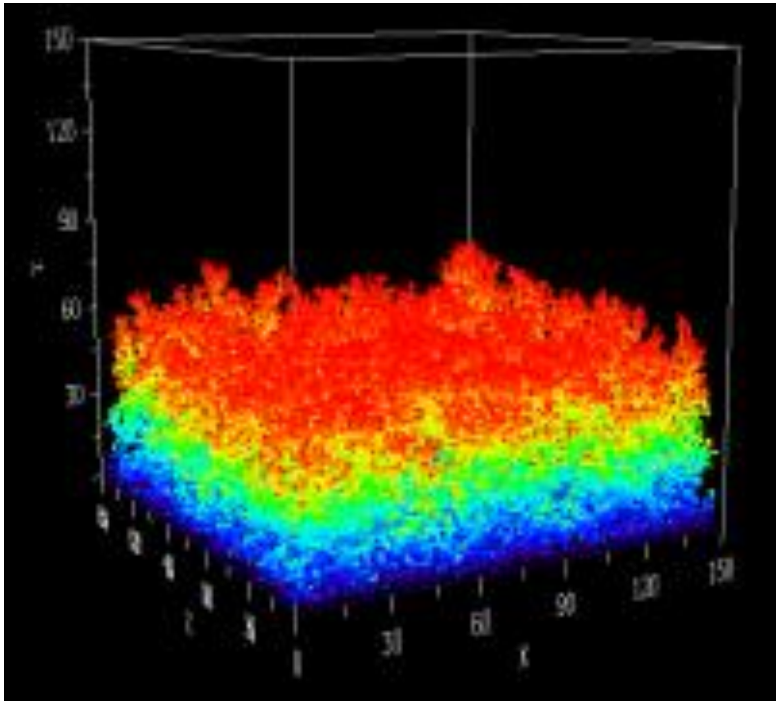
Eden model: Starting from a seed (initial aggregate) the perimeter sites are considered as growth sites. One of them is picked at random and added to the aggregate. There are new born growth sites.

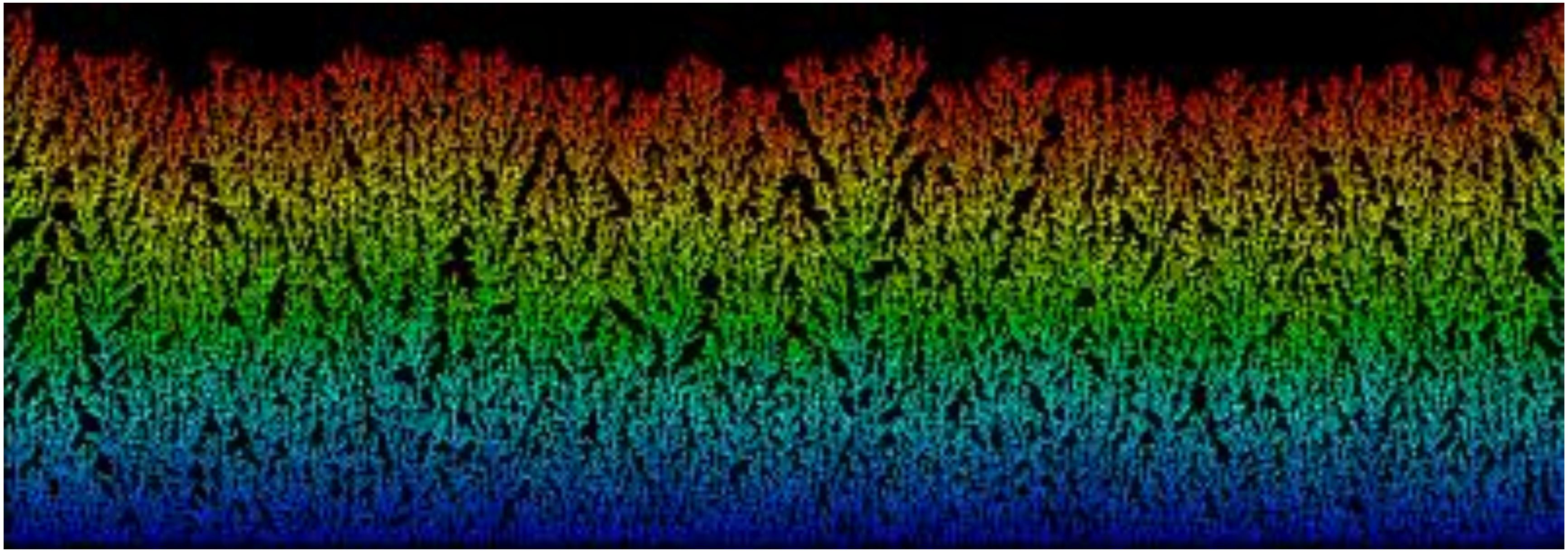


No fractal

Interesting surface

Ballistic deposition





These models lead to objects where $D = d_{embedding}$
Interesting: The structure of the surface**.**
„Surface growth models"
It is more convenient to study them in the „substrate geometry".
The growth starts from a plane d-dimensional substrate and proceeds in the remaining, d+1-st dimension (thus it is called d+1 dimensional growth).
We assume that the surface can be described by a single valued function $h(\mathbf{x})$. This could be identified, e.g., with the maximum distance of the surface above position **x** of the substrate. In these terms the ballistic deposition model reads as:

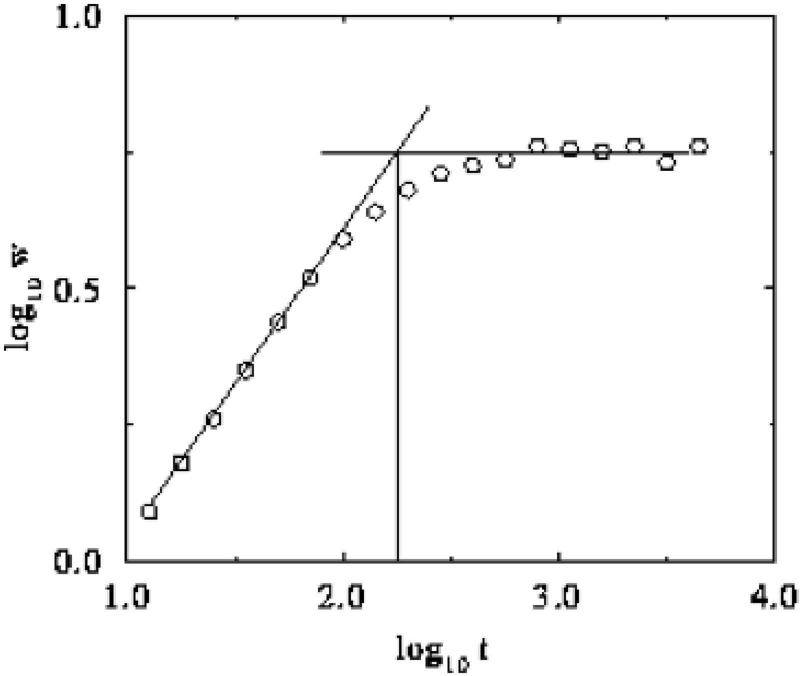
$$h(\mathbf{x},t+1) = \max(h(\mathbf{x},t)+1, h(\mathbf{x}+nn,t))$$

These models lead to non-fractal clusters with constant density. The surface shows interesting scaling behavior.

In the substrate geometry we define a univalued function $h(\mathbf{x})$, which is the position of the surface above the d-dimensional coordinate $\mathbf{x}$ of the substrate. This is not uniquely defined, but the this does not matter as we are interested in scaling.

We define the surface width *w:*

$$w(L,t) = \sqrt{\frac{1}{L}\sum_{i=1}^{L}\left[h(i,t) - \overline{h}(t)\right]^2} \, .$$



For short times we have:

$$w(L,t) \propto t^{\beta} \qquad t \ll t_{\times} \, .$$

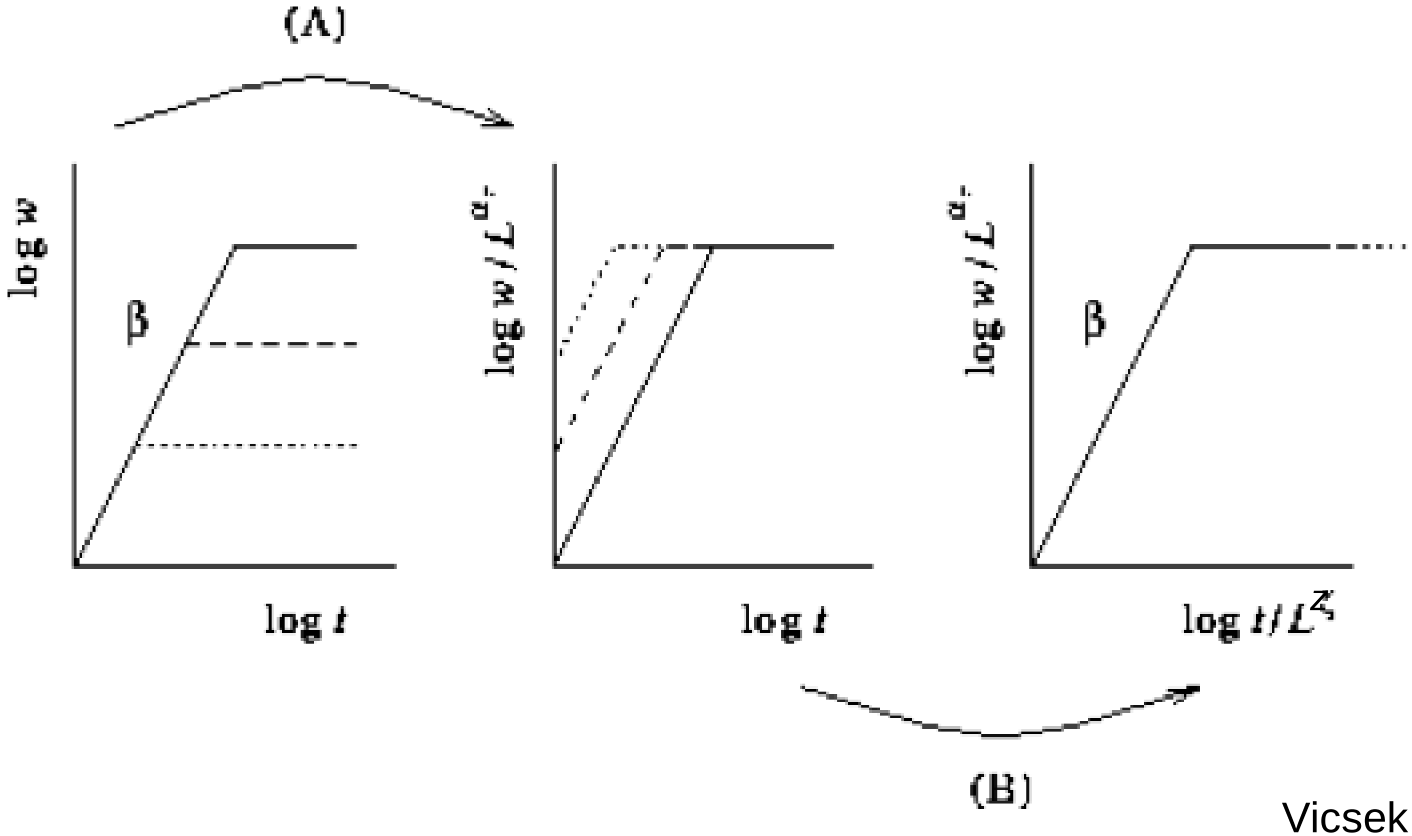
For long times w is independent of t

$$w_s(L,t) \propto L^{\alpha_r} \qquad t \gg t_{\times} \, . \qquad t_{\times} \propto L^{z}$$

These power laws are summarized in a single scaling form:

$w = L^{\alpha} f(t/L^{z})$ $z=\alpha/\beta$

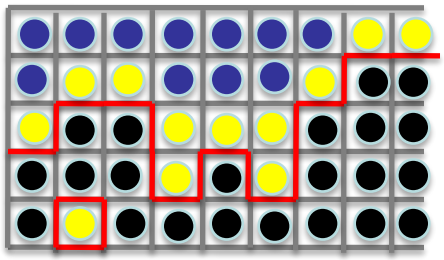
The exponents can – in principle – be determined by „data collapse”

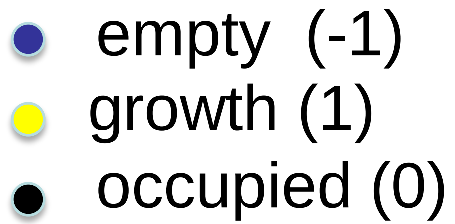


Vicsek and Family, 1985

The Eden model algorithm (square lattice, substrate geometry)

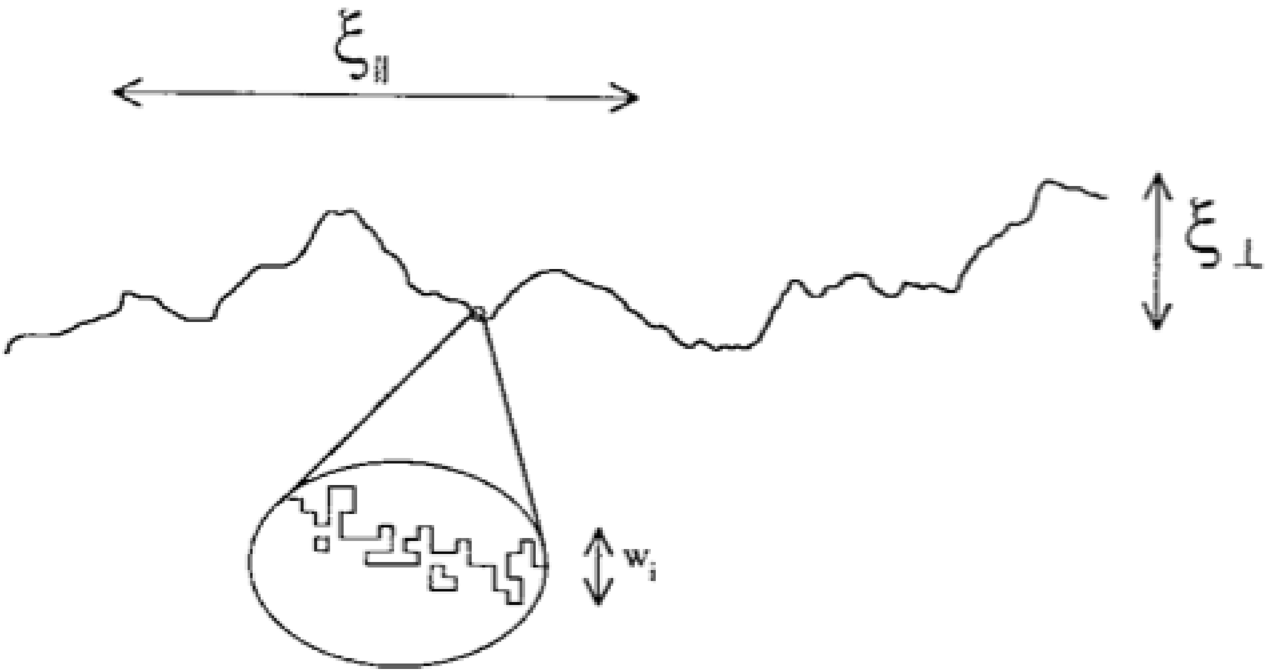
There are 3 kinds of sites: Empty (far from the aggregate), already occupied and growth sites (empty ones with at least on occupied neighbor). In the array *IS* we store the information about the status of the sites. Empty: -1, occupied: 0, growth site: 1. We also store the coordinates of the growth sites in a separate array *IGR*, which has *IP* useful elements, where *IP* = # growth sites.





First an element, say the *I*-th, of *IGR* is picked at random, the *IP*-th element is renamed to the *I*-th and *IP* is set to *IP* -1. *IS* at the selected coordinate is occupied, the empty neighbors become growth sites and the corresponding coordinates are put at the and of the *IGR* list. *IP* is updated accordingly.

As time goes on a characteristic size of surface fluctuations $\xi_\perp(t)$ is buit up over a the substrate region of size $\xi_{||}(t)$, with $\xi_\perp \sim \xi_{||}^{\alpha}$. In reality, for limited samples sizes, the situation is more complicated. Scaling is valid only asymptotically, i.e., for L and $t \rightarrow \infty$ and the „short time" („long time") behavior is meant as $t << t_X$ ($t >> t_X$) For short time/size there are (serious) corrections to scaling. An important source is the structure of the surface.



The long wavelength fluctations show the scaling, while on short scales the local structure (high steps, overhangs, holes) becomes also important. This part of the fluctations contribute to the intrinsic width, where the name shows that locally this quantity would appear as the width of the surface. If we assume that these latter fluctuations are independent of the scaling long wavelength fluctuations, we arrive at the relationship:

$$w^2 = w_i^2 + w_s^2 \qquad (*)$$

where w is the total, w_i is the intrinsic width and w_s is the part, which obeys scaling. As we can measure w the existence of the intrinsic width leads to corrections in scaling. There are several ways to handle this problem:

-Take into account (*), when evaluating scaling. Since w_i is expected to become time and size independent soon, we have

$w^2(2t) - w^2(t) \sim t^{2\beta}$ for the short time behavior.

- Another possibility is to reduce the intrinsic width. This can be done in with the trick of noise reduction as introduced for DLA. Note that there should be a compromise between the gain in scaling and the loss in computing time.
- Analize models, which are in the same universality class (i.e., have the same exponents) as the Eden model but have already very small intrinsic width. Such a model is the so called restricted solid-on-solid model (RSOS). In this lattice model, the surface is indeed a single valued function $h(\mathbf{x})$, where growth happens at randomly selected sites such that the restriction that $|\Delta h| \leq 1$, where Δh is the height difference between neighboring sites.

Using these techniques a large universality class could be identified (ballistic deposition, Eden, RSOS) where the exponents fulfill the scaling law: $\alpha + z = 2$.

The theory of this so called self-affine growth is due to Kardar Parisi and Zhang (KPZ-equation).

Continuum theory of surface growth: an example of stochastic differential equations

We have seen that the scaling behavior of surface growth can be described by a single valued function *h*(**x**,t). Is there an equation of motion for this function?

Due to the fluctuations, this has to be a *stochastic differential equation.*

Differential equation $y'=f(x,y)$ has the solution y(x), i.e., a function. A stochastic d.e. $y'=f(x,y,\eta)$ has the solution $P(y(x))$, where η is the noise. We are often interested only in moments of *y*, like $<y^2>$. The simplest s.d.e. is the Langevin eq. of the Brownian motion (no external force): $\dot{v}(t) = -\gamma v(t) + \eta(t)$, where *v* is the velocity of the Brownian particle, γ is the damping and η the „fluctuating force".

We need to specify *η.* Usually it is assumed to be zero mean, white, Gaussian noise:

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

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

Under these assumptions the above linear sde can be solved.

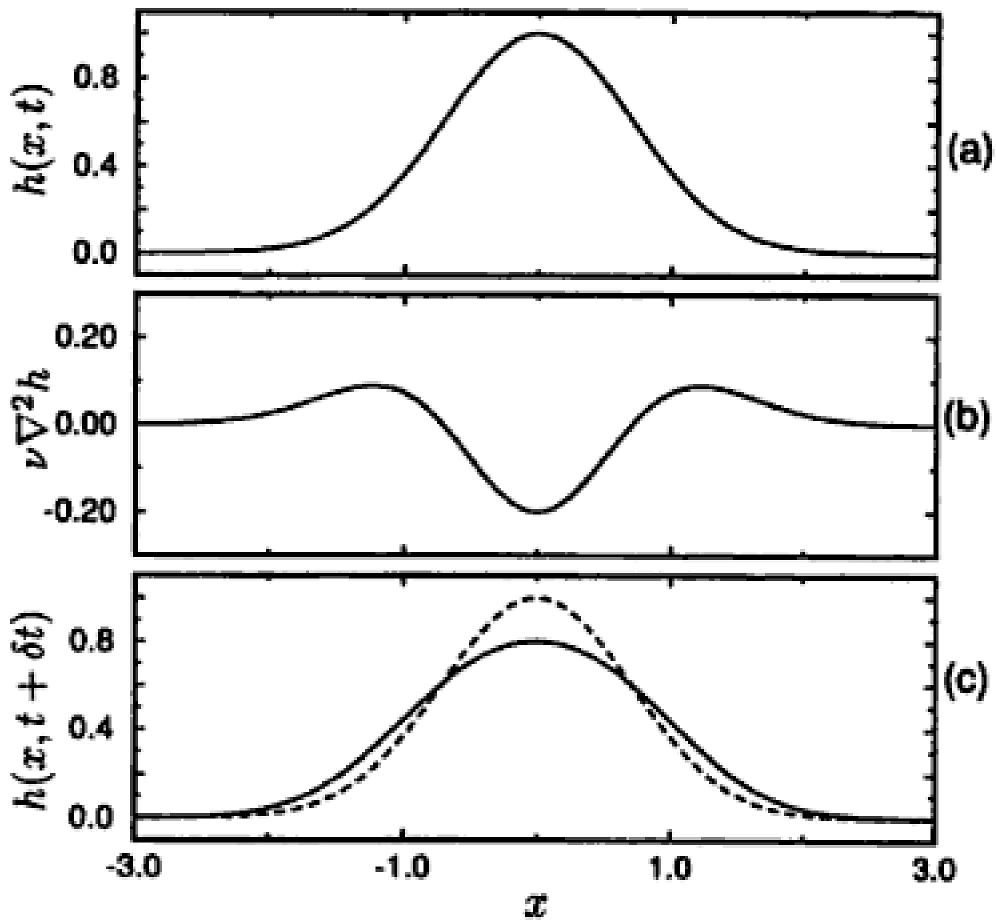
What about surface growth? Since there is a space variable, we look for a stichastic partial differential equation:

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

The simplest such equation is the Edwards-Wilkinson eq.:

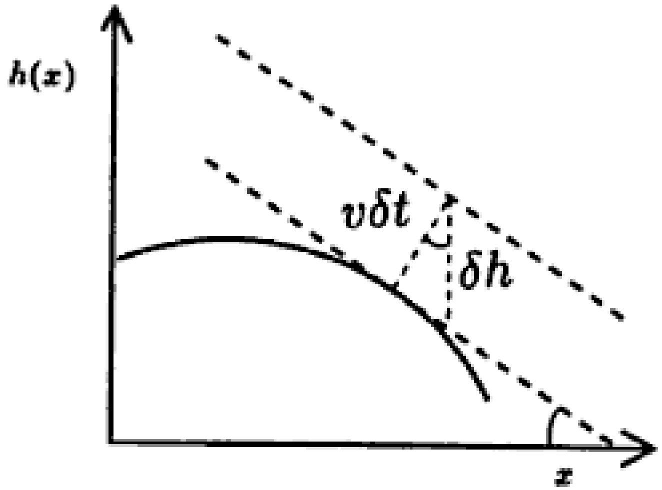
$h(\mathbf{x},t) = \Delta h(\mathbf{x},t) + F + \eta(\mathbf{x},t)$, where *F* is the flux (which can be transformed out using *h*→*h-Ft*). This linear eq. can be solved if *η* is Gaussian white, spacially uncorrelated noise.

The first term is a smoothening one („surface tension”).



The exponents of the EW eq. do not describe the Eden (ballistic deposition etc) models.

In Eden model there is lateral growth:



For small grad *h* this leads to an additional term in the eq., which, after transforming out F has the form:

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

This is the Kardar Parisi Zhang (KPZ) equation, a nonlinear, stochastic, partial differential equation – usually solvable only numerically.

Space discretization (1+1 dimensions):

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

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

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

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

$$\Downarrow$$

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

Treating the noise term (uncorrelated, white):

$$\eta_i(t) = \frac{1}{\Delta x}\int_{x_i-\Delta x/2}^{x_i+\Delta x/2} \eta(x,t)\,\mathrm{d}x$$

with this definition,

$$\langle \eta_i(t) \rangle = 0$$
$$\langle \eta_i(t)\,\eta_j(t') \rangle = \frac{A}{\Delta x}\delta_{ij}\delta(t-t')$$

Time discretization of the noise:

$$W_i(\Delta t) = \int_t^{t+\Delta t} \eta_i(s)ds$$

$$\left\langle W_i(\Delta t)\right\rangle = 0$$

$$\left\langle W_i(\Delta t) W_j(\Delta t)\right\rangle = \int_t^{t+\Delta t} ds' \int_t^{t+\Delta t} ds \left\langle \eta_i(s)\eta_j(s')\right\rangle = \frac{A}{\Delta x}\Delta t \delta_{ij}$$

For solution of the sde we use the Euler scheme (due to stochasticity we do not need that much of precision but be aware of the numerical stability limit: $\Delta t < const.(\Delta x)^z$

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

Handling the last time is difficult (time consuming). If we are interested only in the second moment <$(\Delta h)^2$> then the Gaussian distribution involved can be substituted by a uniform distribution with zero mean and the same variance:

$$h_i(t+\Delta t) = h_i(t) + \frac{\Delta t}{(\Delta x)^2}\left\{\nu\left[h_{i+1}(t) - 2h_i(t) + h_{i-1}(t)\right] + \frac{\lambda}{4}\left[h_{i+1}(t) - h_{i-1}(t)\right]^2\right\} + \sqrt{\frac{A\Delta t}{\Delta x}}\sqrt{12}\left(\xi_i - 1/2\right)$$

where ξ is uniformly distributed on (0,1), thus can be directly taken from a RNG.

Comparison of results (1+1 dimensions)

Exponent	α	β	z
Eden, ballist.	0.5	0.33	1.6
EW	1/2	1/4	2
KPZ	1/2	1/3	3/2

„KPZ” universality class: Far from equilibrium universality

Further algorithmically defined models possible, as empirical circumstances require (MBE). The strategy is similar: Find the appropriate sde and identify the universality class. The universality classes depend on the dimension and the conserved quantities (mass, current).