Simulations in Statistical Physics

Course for MSc physics students

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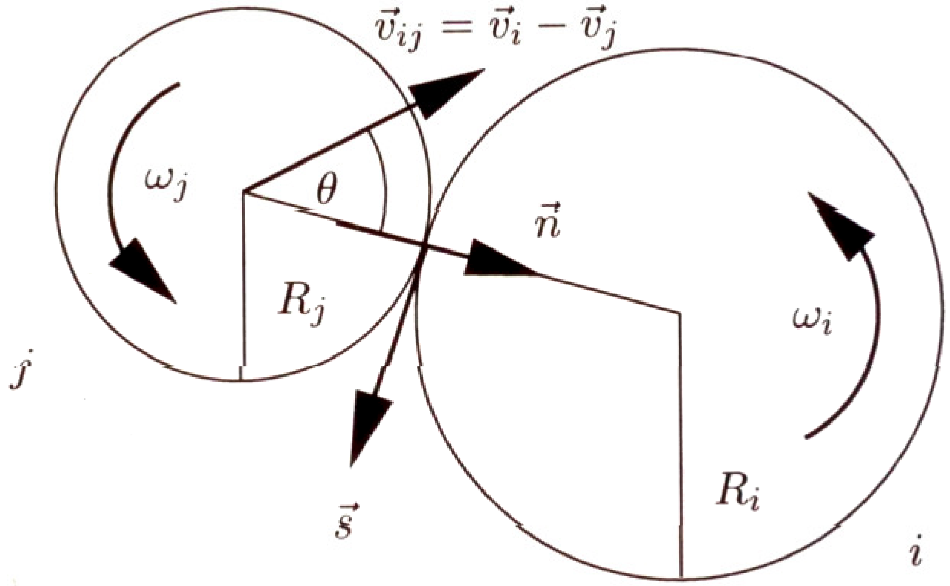
Lecture 11

Simulation of granular material (molecular dynamics = granular dynamics = **distinct element method**)

- Macroscopic particles (have temperature, pressure)
- Short range asymmetric interaction
- Dissipative collisions
- Friction

Rigid particle model: Angular momentum and friction has to be considered

Event driven



Perfect slip (no role of angular momentum)

Define „effective mass“:

$$m_{eff} \equiv \frac{m_i m_j}{m_i + m_j}$$

$$\overrightarrow{\Delta p_n} = -2m_{eff}\left[\left(\vec{v}_i^{\,before} - \vec{v}_j^{\,before}\right)\vec{n}\right]\vec{n}$$

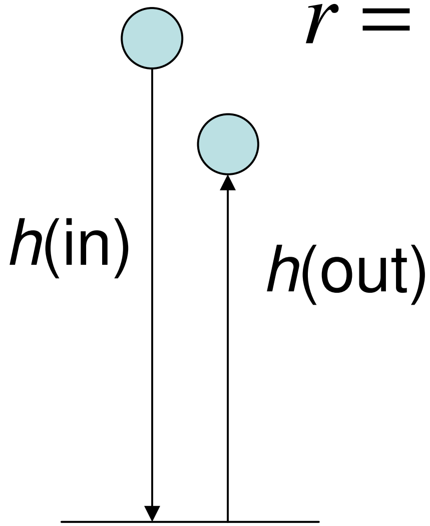
$$\vec{v}_i^{\,after} = \vec{v}_i^{\,before} - \frac{\overrightarrow{\Delta p_n}}{m_i} \quad , \quad \vec{v}_j^{\,after} = \vec{v}_j^{\,before} + \frac{\overrightarrow{\Delta p_n}}{m_j}$$

For stick condition conservation of angular momentum has to be considered

Inelastic collisions are characterized by the **restitution coefficient**

$$r = \frac{h(out)}{h(in)}$$

$$r = \frac{E(out)}{E(in)} = \left(\frac{v(out)}{v(in)}\right)^2 = e_n^2$$

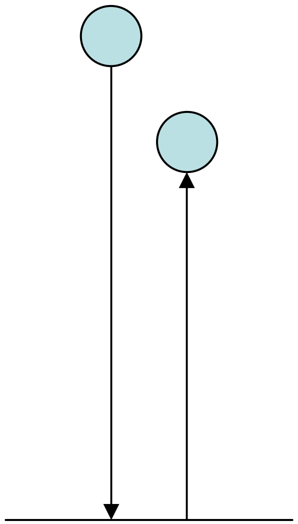


Similarly, a coefficient for the tangential component can be introduced.

$$\left(\mathbf{v}_j^{after} - \mathbf{v}_i^{after}\right)\cdot \mathbf{n} = -e_n \left(\mathbf{v}_j^{before} - \mathbf{v}_i^{before}\right)\cdot \mathbf{n}$$

$$\Delta \mathbf{p} = -m_{eff}\,(e_n + 1)\left[\left(\mathbf{v}_j^{before} - \mathbf{v}_i^{before}\right)\cdot \mathbf{n}\right]\cdot \mathbf{n}$$ for perfect slip

Finite time singularity (inelastic collapse: numerical instability):



How long does it take until it stops?

$$t_{tot} = \sum_j t_j = 2\sqrt{\frac{2h^{initial}}{g}} \sum_j \sqrt{r^j} = 2\sqrt{\frac{2h^{initial}}{g}} \left(\frac{2}{1-\sqrt{r}} - 2 \right)$$

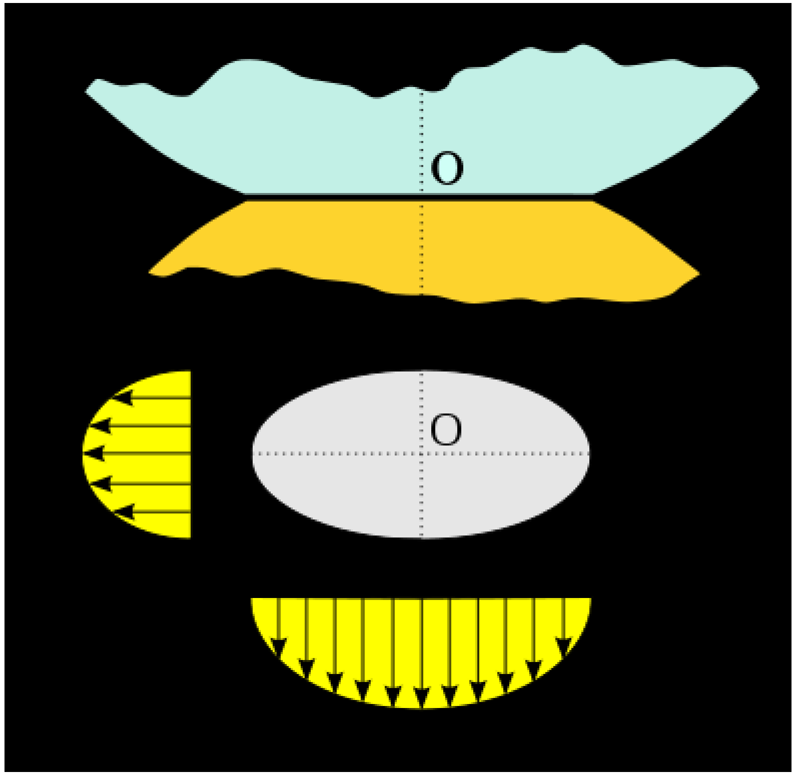
∞ number of collisions in finite real time.
Event driven simulation does not work.

http://www.haverford.edu/physics-astro/Gollub/vib_granular/inelastic/inelastic.html

Ways out:
- Change *r* with the velocity (physics) $r \sim (\Delta v)^{1/5}$
- Use soft potential and time steps
- Use different technique (Contact Dynamics)

Soft potential with finite time steps

Viscoelastic model: $$F = \theta(-x)(-kx - \gamma\dot{x})$$



Hertzian contact: Even material with linear properties will be nonlinear. For pure elasticity:

$$F_n^{elastic} = A\xi^{3/2}\theta(\xi)$$

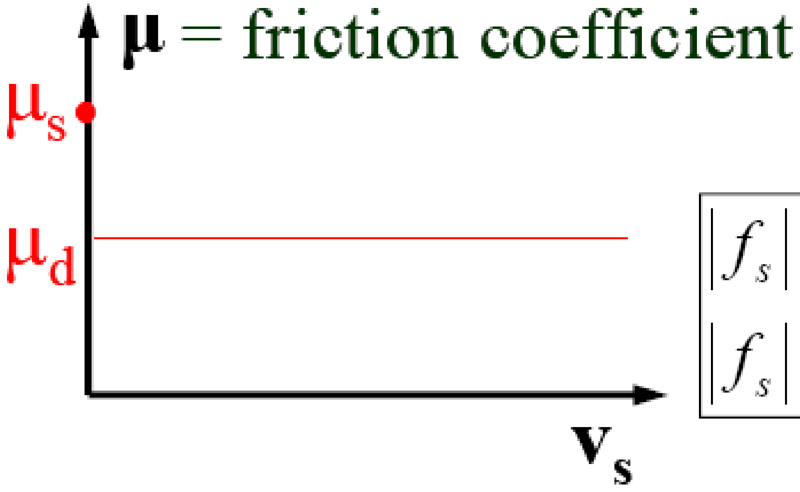
Where *A* depends on the elastic moduli and the particle radius.

$$F_n^{diss} = B\sqrt{\xi}\,\dot{\xi}\theta(\xi)$$

B determines *r*

Similar, more complicated expressions are valid for F_t

Coulomb friction with rigid particles:



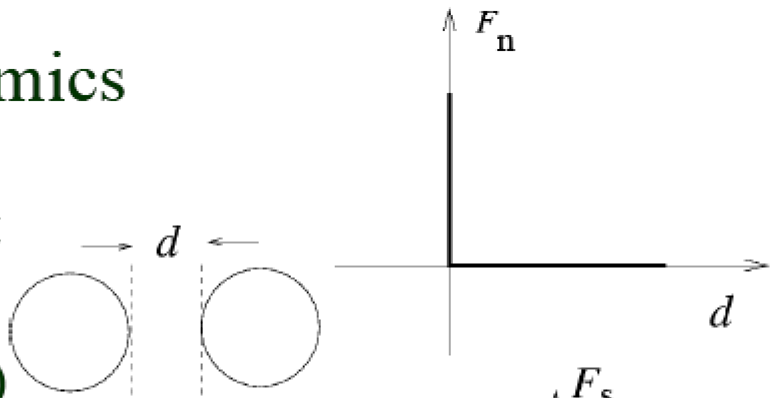
$$
\begin{array}{|llll|}
\hline
|f_s| \leq \mu_s |f_n| & \text{if} & v_s = 0 & \\
|f_s| \leq \mu_d |f_n| & \text{if} & v_s \neq 0 & \\
\hline
\end{array}
$$

static case

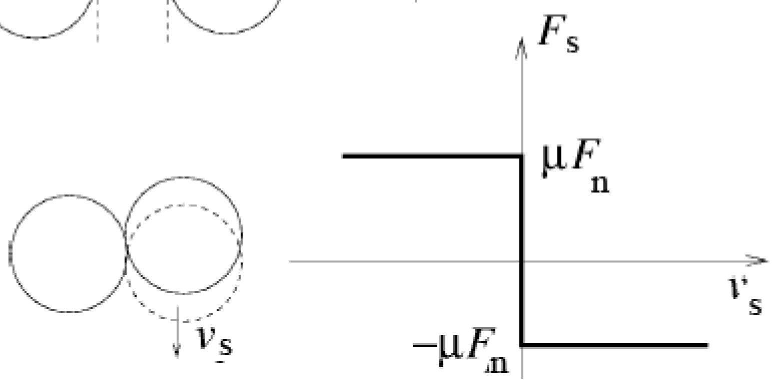
dynamic case

Non-smooth dynamics

Signorini-Graph: perfect volume exclusion (perfectly rigid particles)



Coulomb-Graph: friction between particles with relative tangential velocity v_s



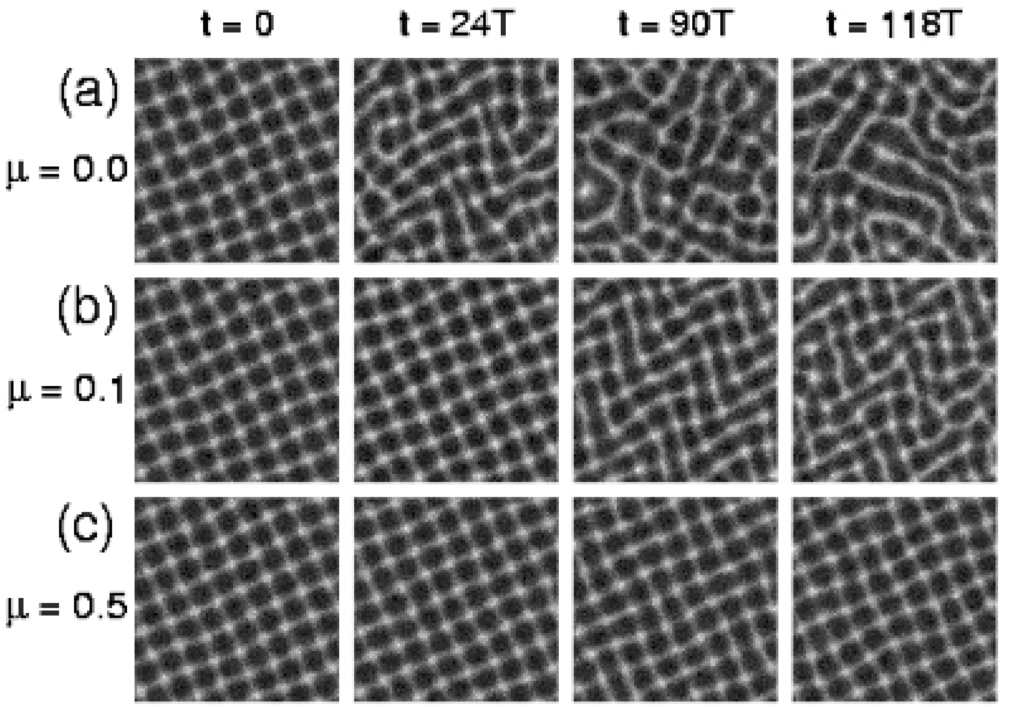
Contact dynamics

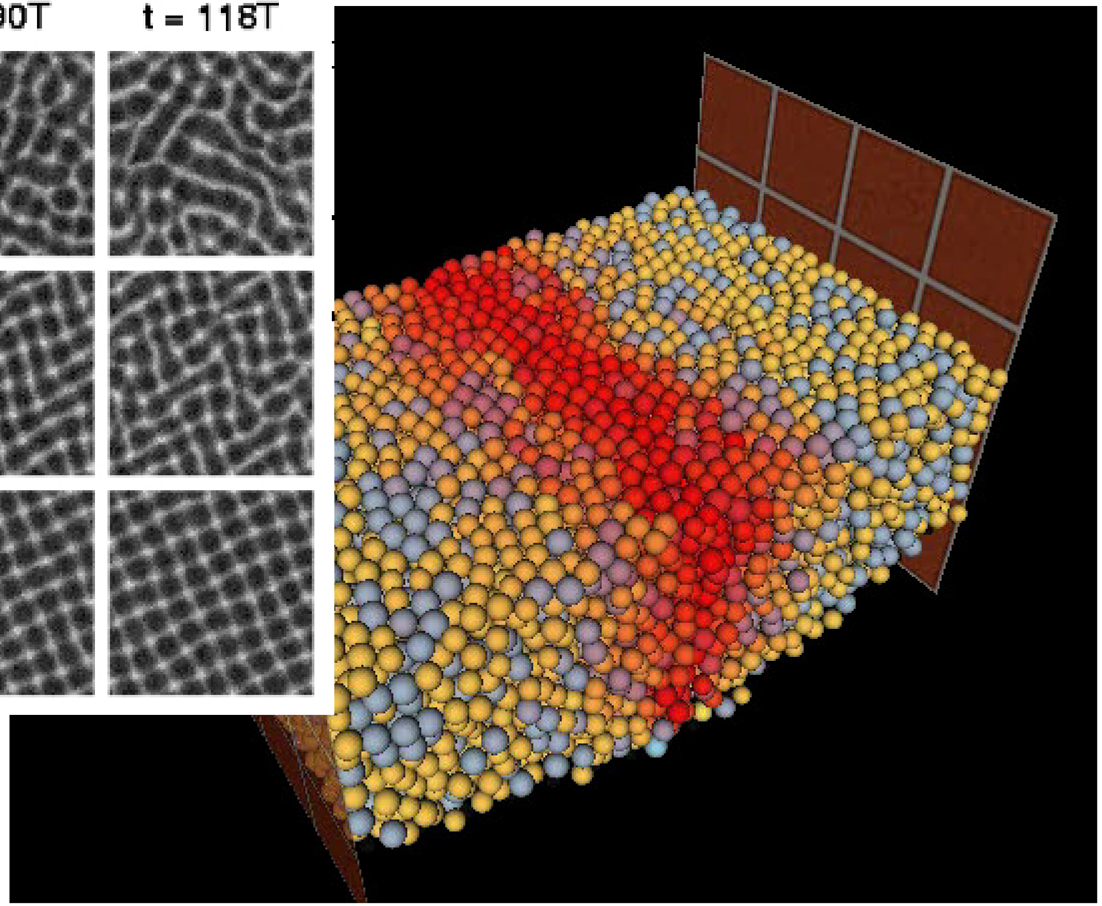
Shear

http://www.ph.biu.ac.il/~rapaport/java-apps/grshear.html

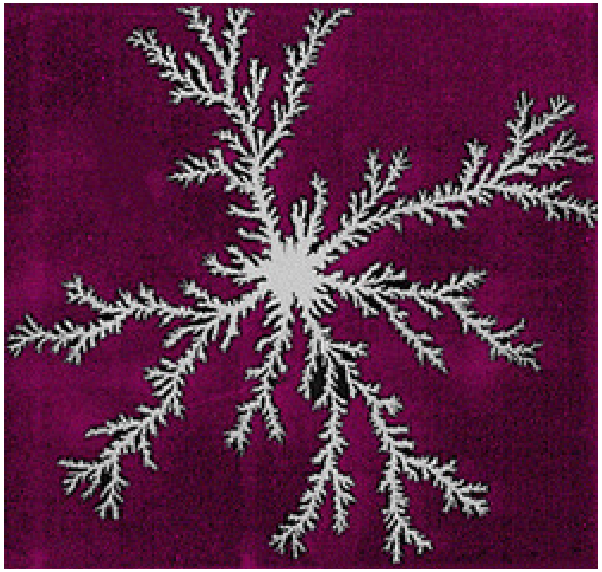
Vibrating plate

http://www.ph.biu.ac.il/~rapaport/java-apps/grvib.html



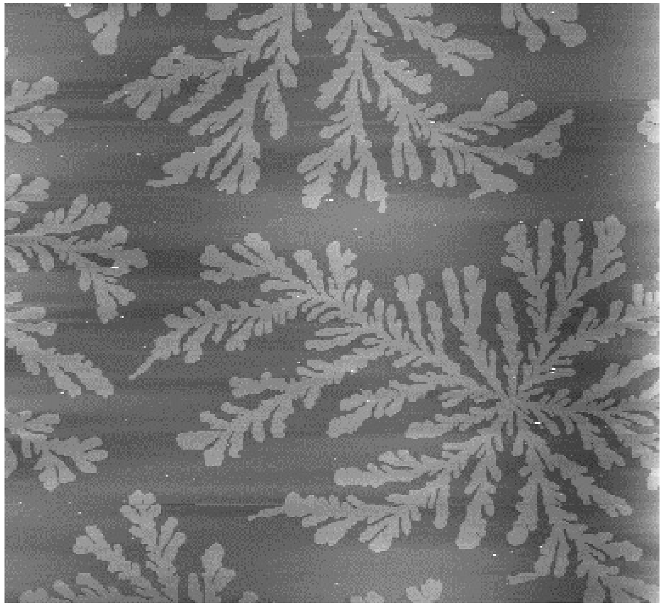


Algoritmikusan definiált modellek: Fraktál növekedés

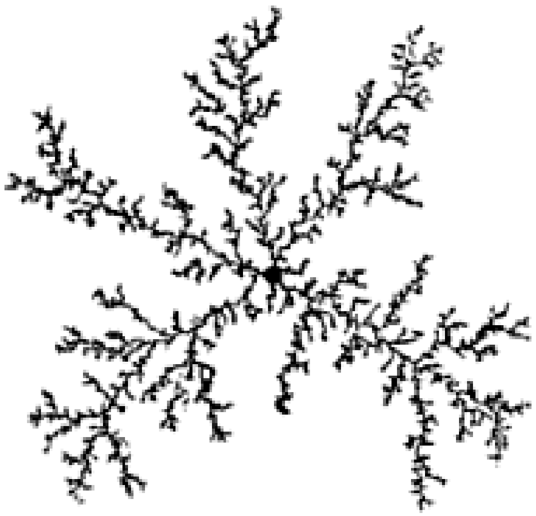


Elctrochem. deposition

Mineralization

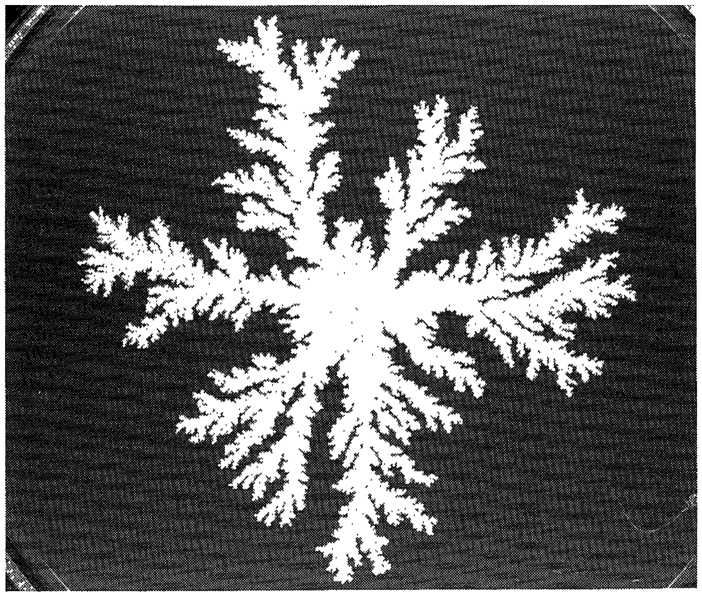


Surface crystallization



Disordered viscous fingering

Bacterial colony growth



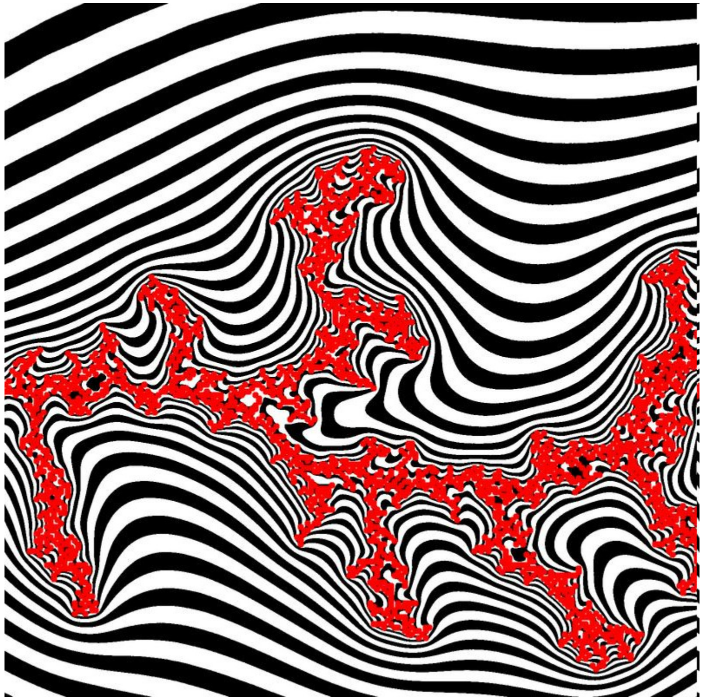
Basic equations:

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

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

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

$$+ \text{ disorder}$$



Laplacian or gradient governed groth:

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

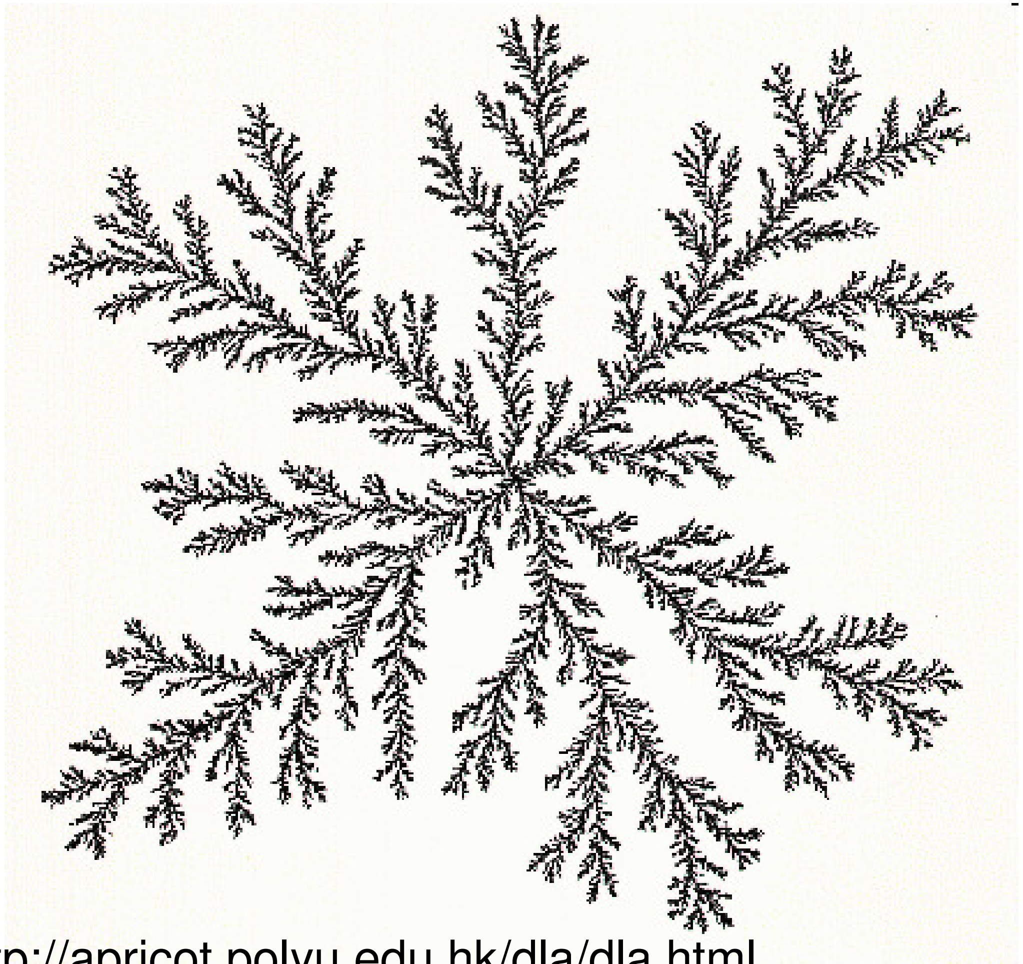
+ screening:
If 2 bumps grow, the faster will screen the slower and stop its growth

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 *

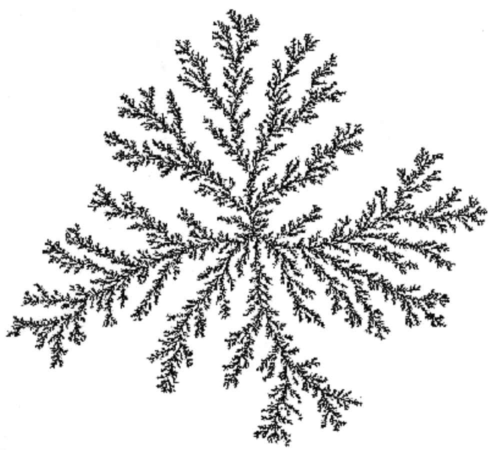


http://apricot.polyu.edu.hk/dla/dla.html

100 million particles

Coarsened

Self-similar structure



1 million particles

In order to simulate (relatively) large samples tricks are needed

- No need to start from infinity: 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)

Why are so terribly large aggregates needed?

Self similar fractals, scaling → asymptotic behavior

How to measure fractal dimension?

Dimensions

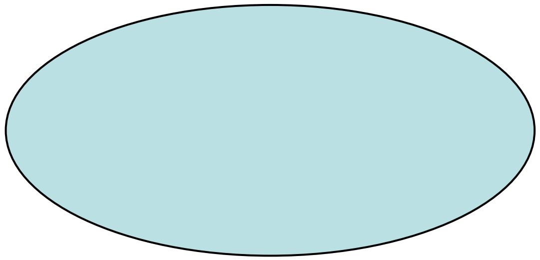
- Topological dimension:

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

- Embedding dimension:

Number of independent directions

- Hausdorff (fractal) dimension



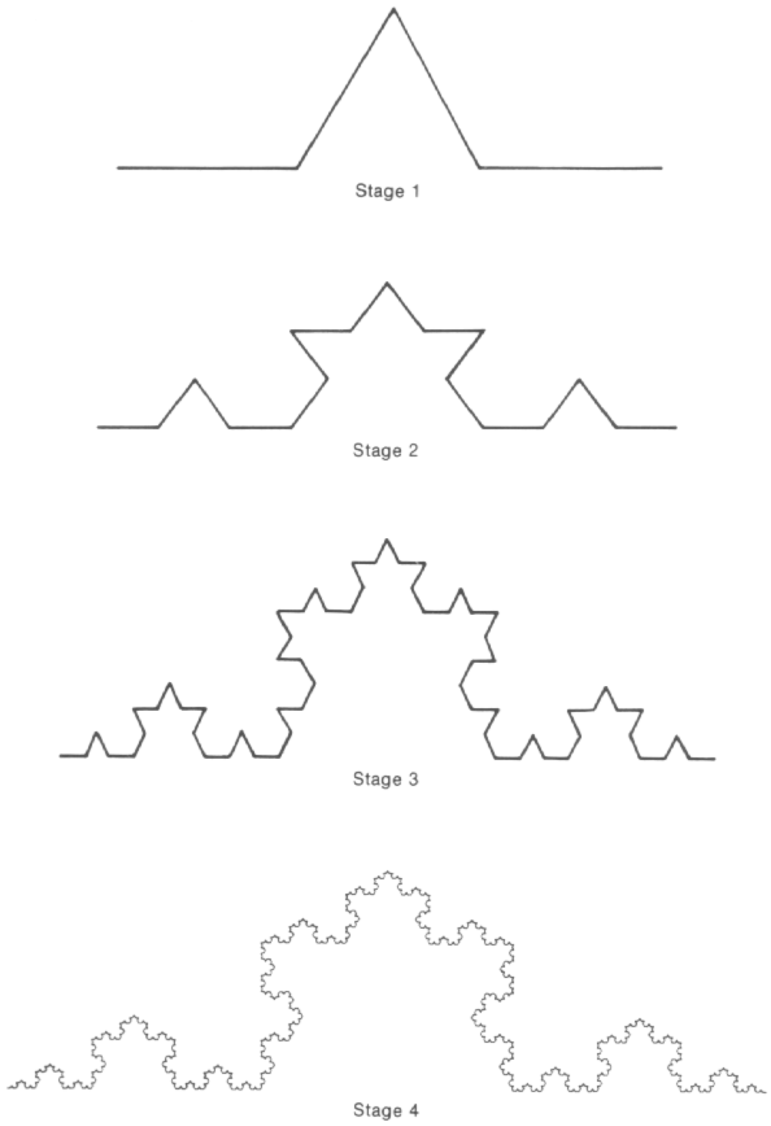
Area *A* is mesured by covering the object with squares of size ℓ^2. # of such boxes: N_ℓ.

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

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

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.*

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

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

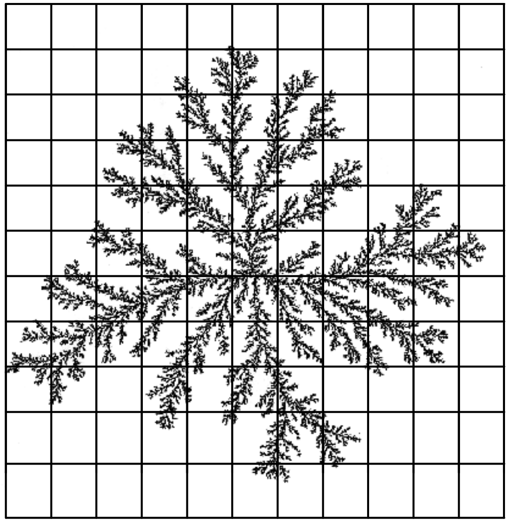
Instead of using d_t find the appropriate D fractal dimension such that

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

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

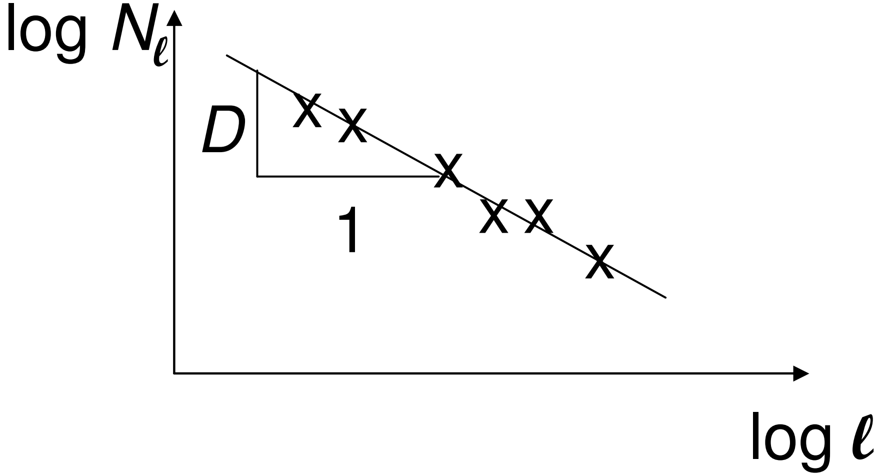
(Def of fractal: $d_t < D < d_e$)

How to measure D for a random fractal?

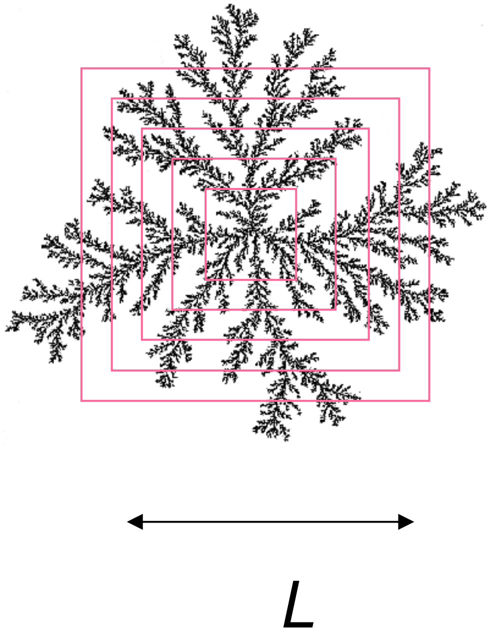


There is always a lower and an upper cutoff (e.g., particle size, radius of gyration).

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

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

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

$$D = d - \alpha$$