Cooperative and critical phenomena

Outline

- Growth, self aggregation, gelation.
- Percolation theory.
- Surface growth and the KPZ equation.
- Collective behavior: Flocking, swarming and herding.

- # Growth, self aggregation, gelation

Understanding the development of different morphologies in physical, chemical and biological systems has provided one of the main motivations for the study of non-equilibrium growth models.

Much of the present understanding of non-equilibrium growth results from computer simulations using simple models.

Growth models

- DETERMINISTIC (Cellular automata)
- PROBABILISTIC

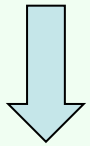
The structure is often characterised by its fractal dimensionality *D* (*d* is the euclidean dimension)

Mass: $M \sim l^D$

Two-point density correlation: $c(r) \sim r^{D-d}$

Growth models:

1. The EDEN model.
2. Diffusion/reaction limited aggregation.



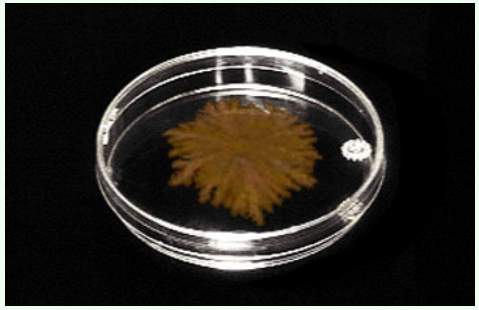
LAPLACIAN GROWTH

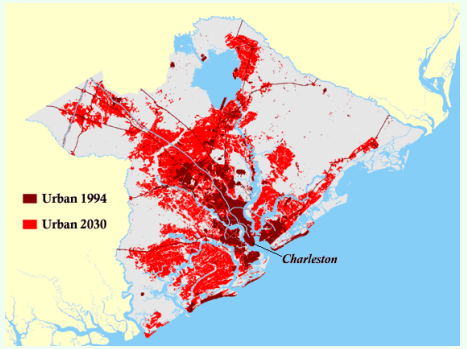
3. Additional examples.

1. The EDEN model (Murray Eden 1961)

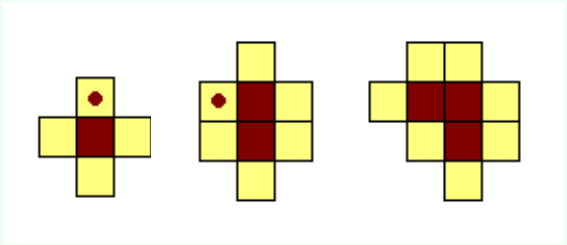
Motivation: Description of the growth of clusters of bacteria colonies and the random accumulation of materials deposited on the boundaires.

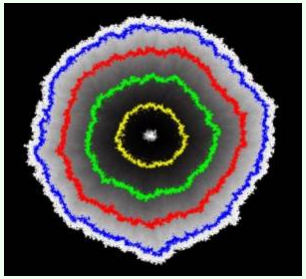
Applied to tumor growth, urban develoment, the formation of snowflakes…





The model





Prob placing particle N at a distance r from the cluster CM:

$$P(r,N) = \frac{1}{\sqrt{2\pi}\sigma_N} \exp\left[-\frac{(r-\bar{r}_N)^2}{2\sigma_N^2}\right]$$

$$\bar{r}_N = \langle \sum_i r_N(i) \rangle \sim N^{0.495 \pm 0.005}$$

Width of the active zone:

$$\sigma_N = \left\langle \sum_i (r_N(i) - \bar{r}_N)^2 \right\rangle^{1/2} \sim N^{0.18 \pm 0.03}$$

The radius of gyration:

$$R_g = \left\langle \sum_i (r_i - r_{CM})^2 \right\rangle^{1/2} \sim N^{0.5}$$

Michael Plischke and Zoltán Rácz Phys. Rev. Lett. **53**, 415 (1984)

An application to skin cancer

Williams, T., Bjerknes, R. Nature, 236, 19 (1972)

Rules:

- Conseider a triangular lattice
- Cells: (0=normal/unoccupied; 1=cancerous)
- Start with a single cancerous cell
- Select a lattice site (a) located in either the occupied or the unoccupied perimeter
- Select (b), a nn site of (a)
- Assign to (b) the label of (a)

Introducing growth limitations:

C. S. Ferreira, Physica A, 317,565-580 (2003)

- Mutation probability:

g: $N \to T$

r=1-g: $T \to N$

- Carcinogenic advantage: $\kappa = \frac{g}{1-g}$ $\quad g = \frac{\kappa}{\kappa+1};\ r = \frac{1}{\kappa+1}$

Eden model $\kappa \to \infty$

Ferreira introduced a new model assuming the probabilities to depend on the number of tumor cells n
(Michaelis Mentem functions)

$$g(n) = 1 - \frac{\alpha n}{\Gamma + n}$$

$$r(n) = \frac{\alpha n}{\Gamma + n} \qquad 0 < \alpha < 1;\ \Gamma > 0$$

- Since *g(n)* and *r(n)* are time independent, any given pattern in a certain time depends only on the configuration at the previous time (Markov chain).

- The growth process can be described within the framework of a probability transition or master equation.

$$P(n, t+1) = \sum_m T_{n,m} P(m.t)$$

Probability of a state with n tumor cells at t+1

Transition matrix

$$T_{n,m} = \begin{cases} g(n), & \text{if } n = m+1; \\ r(n), & \text{if } n = m-1; \\ 0, & \text{if } |n-m| > 1. \end{cases}$$

Valid for $n \geq 2$
n=0 absorbent state
$T_{0,1}$= r; $T_{1,0}$= 0

$$\begin{cases} P(n,t+1) = gP(n-1,t) + rP(n+1,t), & \text{if } n \geq 2 \\ P(n,t+1) = rP(n+1,t), & \text{if } n = 0,1 \end{cases}$$

From the previous equations we can evaluate the number of tumor cells and its variance

$$\langle n(t) \rangle = \sum_{n=0}^{\infty} nP(n,t)$$

$$\left\langle n^2(t) \right\rangle = \sum_{n=0}^{\infty} n^2 P(n,t)$$

$$\sigma^2(t) = \left\langle n^2(t) \right\rangle - \langle n(t) \rangle^2$$

$$\langle n(t) \rangle = n(0) + \frac{\kappa - 1}{\kappa + 1} t$$

$$\sigma^2(t) = \left[1 - \left(\frac{\kappa - 1}{\kappa + 1} \right)^2 \right] t$$

A continuous approach:

$$\frac{d}{dt} P(n,t) = \sum_{m \neq n} \left[W_{n,m} P(m,t) - W_{m,n} P(n,t) \right]$$

$$W_{n,m} = \begin{cases} g(m), & \text{if } n = m+1; \\ r(m), & \text{if } n = m-1; \\ 0, & \text{if } |n-m| > 1. \end{cases}$$

$$\frac{d}{dt}P(n,t) = g(n-1)P(n-1,t) + r(n+1)P(n+1,t) - P(n,t)$$

$$\frac{d\langle n(t)\rangle}{dt} = 1 - 2\alpha\left\langle \frac{n(t)}{\Gamma + n(t)} \right\rangle$$

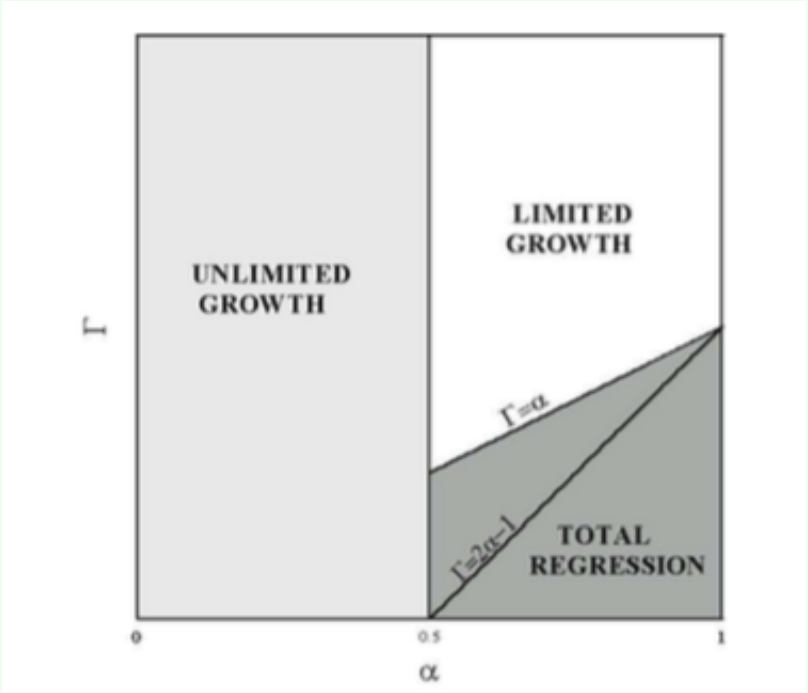
$$\frac{d\langle n^2(t)\rangle}{dt} = 1 + 2\left\langle \frac{n(t)[\Gamma + (1-2\alpha)n(t)]}{\Gamma + n(t)} \right\rangle$$

Mean field approach:

$$\langle n(t)\rangle \to N(t)$$

$$\frac{dN(t)}{dt} = 1 - 2\alpha\frac{N(t)}{\Gamma + N(t)}$$

$$\frac{dN^2(t)}{dt} = 1 + 2\frac{N(t)[\Gamma + (1-2\alpha)N(t)]}{\Gamma + N(t)}$$



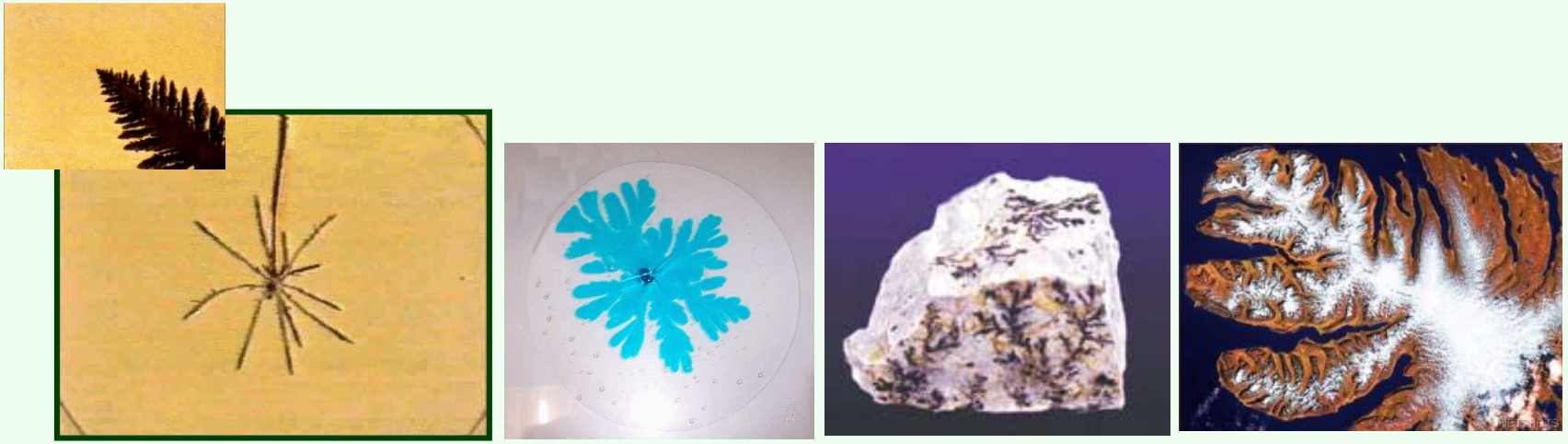
2. Diffusion/Reaction Limited Aggregation DLA/RLA

Describes a process in which particles perform a random walk due to brownian motion and cluster together to form aggregates.

Diffusion is the primary means of transport and the limiting growth factor.

Examples:

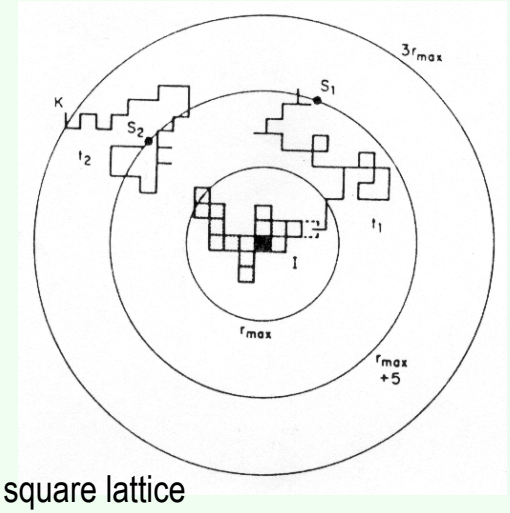
- Electrodepostion
- Hele-Shaw flow
- Mineral deposits
- Glaciars
- Tissue growth controlled by the diffusion of nutrients and toxic metabolites



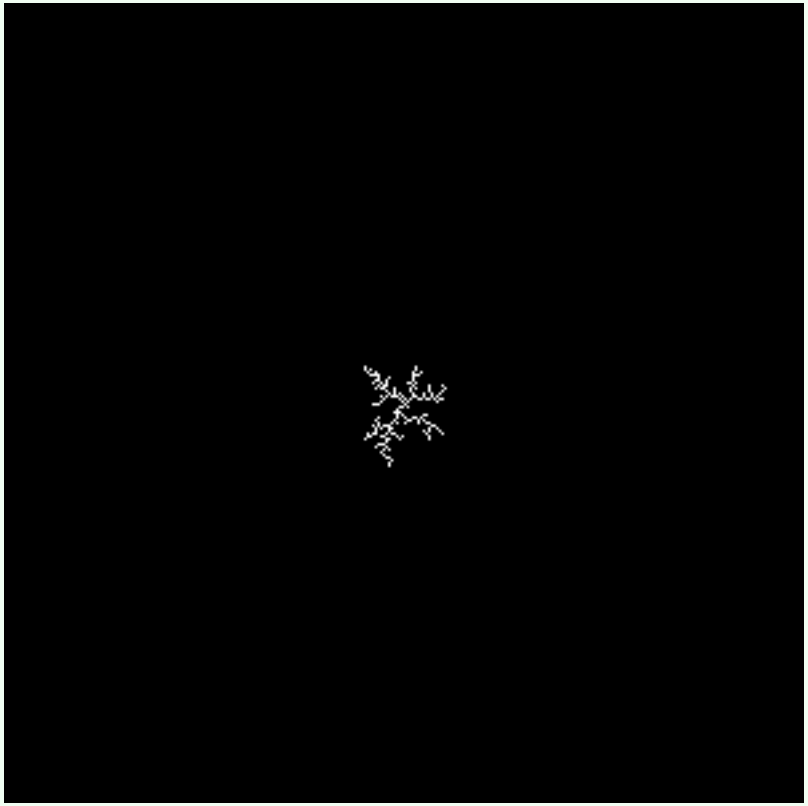
See 3d DLA animation from the web
https://www.youtube.com/watch?v=h3O1LGe-dBw

The model

T. A. Witten, Jr. and L. M. Sander Phys. Rev. Lett. **47**, 1400



2-d square lattice



The radius of gyration: $R_g \sim N^{1/D}$

$$D \approx 1,7$$

$$C(r) \sim r^{D-d} = r^{-0,343}$$

Random walker
P(i,j;t)=[P(i-1,j;t-1) + P(i+1,j;t-1) + P(i,j+1;t-1) + P(i,j-1;t-1)]/4

$$\nabla^2 P = 0$$

The dielectric breakdown model

Niemeyer et al, Phys. Rev. Lett, 52, 1033 (1984)

$$\nabla \cdot \vec{E} = \frac{\rho}{\epsilon}$$

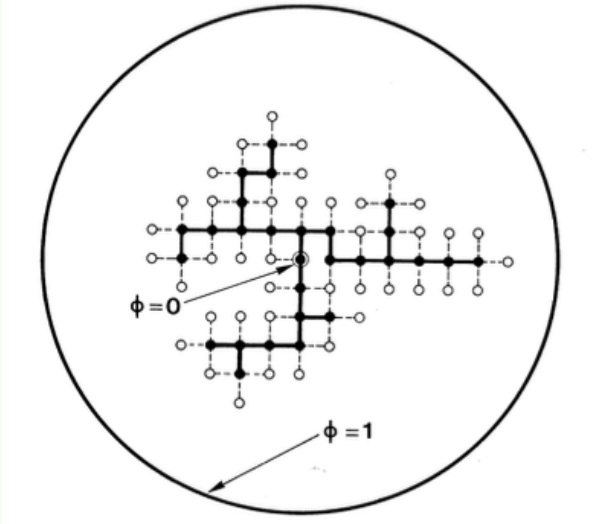
$$\vec{E} = -\nabla V$$

$$\nabla^2 V = -\frac{\rho}{\epsilon}$$

Dielectric media: $\nabla^2 V = 0$

V(i,j;t)=[V(i-1,j;t-1) + V(i+1,j;t-1) + V(i,j+1;t-1) + V(i,j-1;t-1)]/4

The model



$\eta = 1; D = 1.75 \pm 0.02$

Propagation depends on the strength of the electric field.

With appropiate boundary conditions

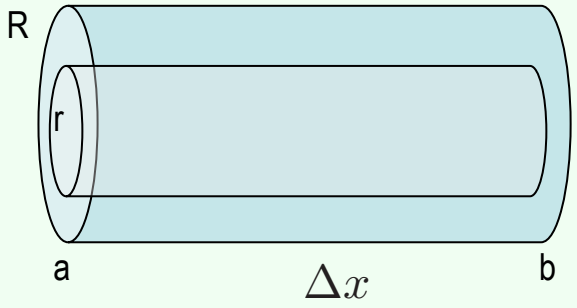
$$\vec{E}(i,j \to i\prime,j\prime) \propto V_{i\prime,j\prime}$$

$$p(i,j \to i\prime,j\prime) = \frac{(V_{i\prime,j\prime})^\eta}{\sum_{[i\prime,j\prime]}(V_{i\prime,j\prime})^\eta}$$

A scalar field that obeys the Laplace equation can be represented by a radom walk.

Eden model $\eta = 0$

3. Additional examples



- Fluid flow through a pipe

$$F_P = \Delta P dA$$

$$F_{\mu,fast} = -\mu 2\pi r \Delta x \left.\frac{\partial u}{\partial r}\right|_r$$

$$F_{\mu,slow} = \mu 2\pi (r+dr) \Delta x \left.\frac{\partial u}{\partial r}\right|_{r+dr}$$

$$0 = F_P + F_{\mu,fast} + F_{\mu,slow}$$

$$\Delta P 2\pi r dr - \mu 2\pi r \Delta x \left.\frac{\partial u}{\partial r}\right|_r + \mu 2\pi (r+dr) \Delta x \left.\frac{\partial u}{\partial r}\right|_{r+dr} = 0$$

$$\left.\frac{\partial u}{\partial r}\right|_{r+dr} = \left.\frac{\partial u}{\partial r}\right|_r + \left.\frac{\partial^2 u}{\partial r^2}\right|_r dr$$

$$-\frac{1}{\mu}\frac{\Delta P}{\Delta x} = \frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) = \nabla^2 u$$

Poiseuille flow:

$$u(r) = \frac{1}{4\mu}\frac{\Delta P}{\Delta x}(R^2 - r^2)$$

No-slip boundary condition at the wall: $u(r) = 0; r = R$

Axial symmetry: $\frac{du}{dr} = 0; r = 0$

Incompressible fluid:

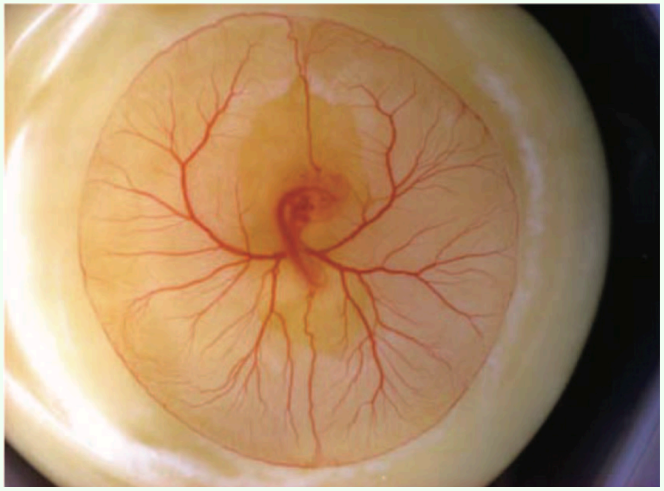
$$\nabla \cdot u(r) = 0 \rightarrow \nabla^2 P = 0$$

Application to vascular morphogenesis

The growth of arteries and veins follows the directions of high shear stress provoked by the blood flow on the endothelial wall of a pre-existing capillary mesh.

Additional requirements:

- Disconnection of small side branches.
- Reconnection of dangling sprouts.
- Plastic extension of the interstitial tissue



Thi-Hanh Nguyen et al.
Dynamics of vascular branching morphogenesis: The effect of blood and tissue flow
PHYSICAL REVIEW E **73**, 061907 2006

Self aggregation and gelation:

1. Self-assembly: a common process in Nature.

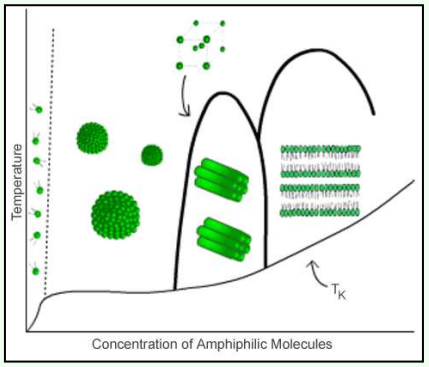
2. Growth kinetics of the self-assembly process.
   The DLCA model
   The mean field Smoluchowski equation

1. Self-assembly: a common process in Nature

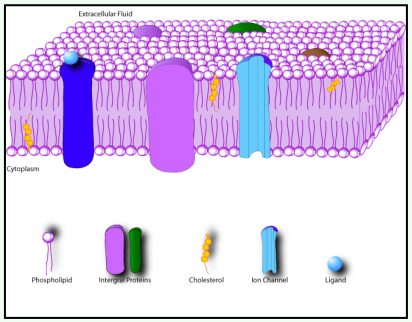
Self-assembly is a natural phenomenon that can be observed in many biological, chemical and physical processes, in which the cell is, perhaps, the ultimate supramolecular structure comprising many millions of molecules held together by weak non-covalent chemical forces, particularly hydrogen bonds and hydrophobic interactions.

Self-assembling of amphiphilic molecules

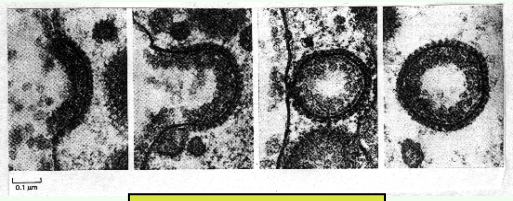
Lyotropic liquid crystals



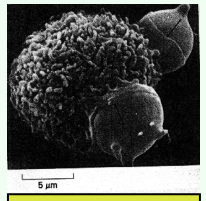
Fatty acids (phospholipids, glycolipids, cholesterol)



Cell membrane composition provides exceptional mechanical properties

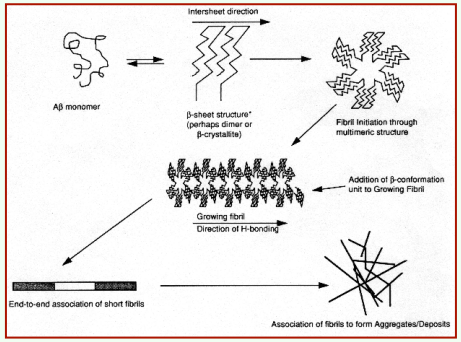


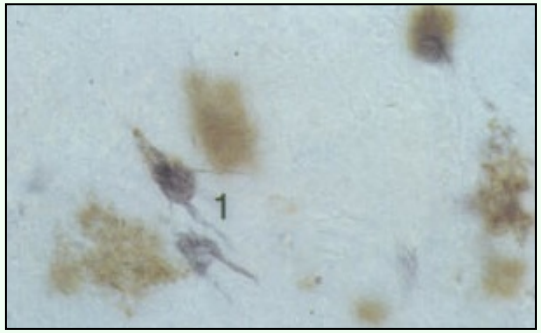
Endocytosis



Phagocytosis

Azheimer disease

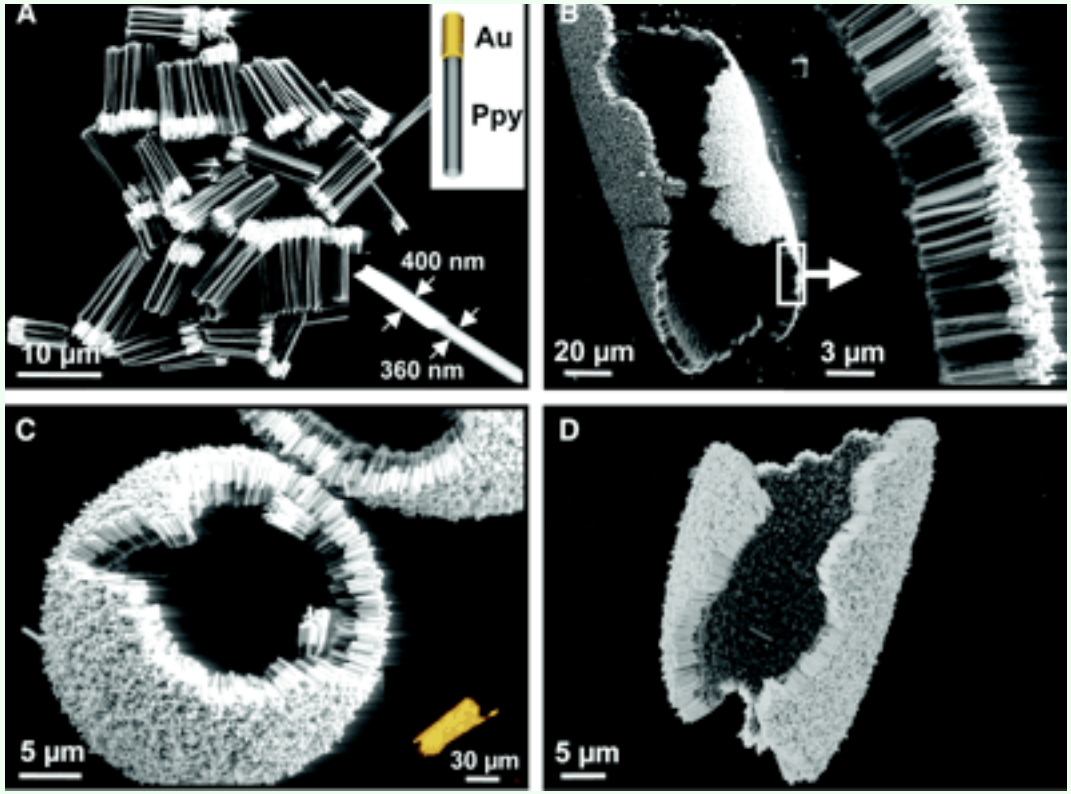




From PNAS, 87, 3947, (1990)

- Aβ fragments generated due to overexpressing mutant forms of its APP, are toxic to neurons, self-aggregate becoming insoluble structures.
- Fibrous protein aggregates can be made in vitro with widths in the nanometer and lengths in the micrometer Range. These structures are resistent to harsh conditions

Self-assembling of metal - polymer amphiphiles

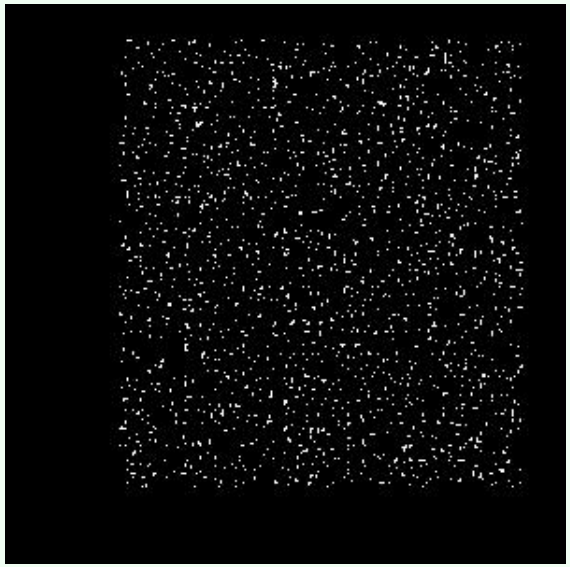


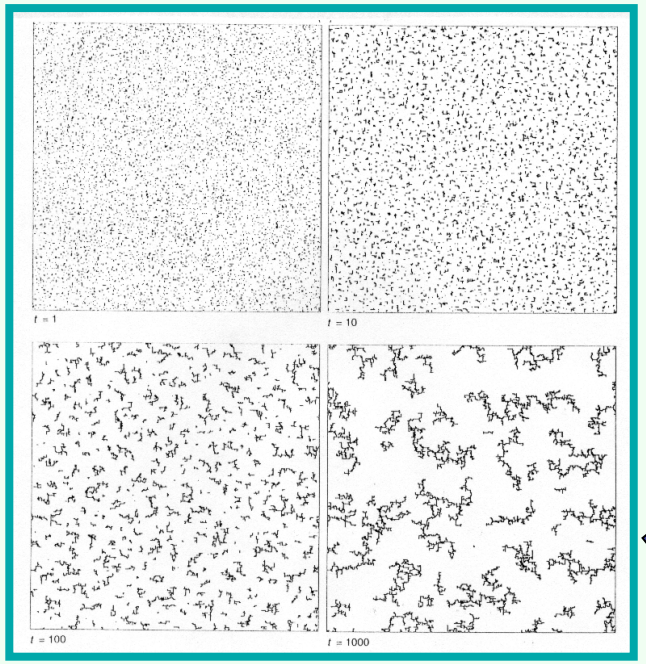
From Science, 303 (5656), 348 (2004).

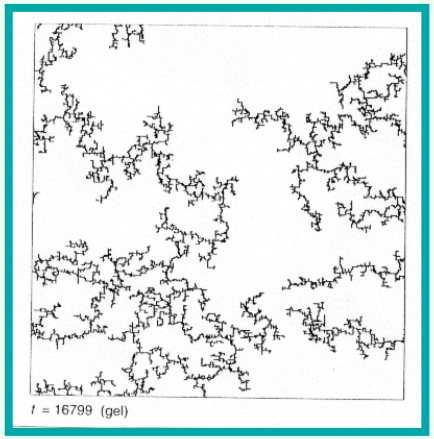
Segmented metal-polymer rods were prepared by electrodeposition of gold into porous aluminum templates followed by electrochemical polymerization of pyrrole. The length of each block is controlled by monitoring the charge passed during the electrodeposition process. Different structures are found depending on the block size ratio Au:Ppy.

(B) 1:4; (C) 3:2; (D) 4:1.

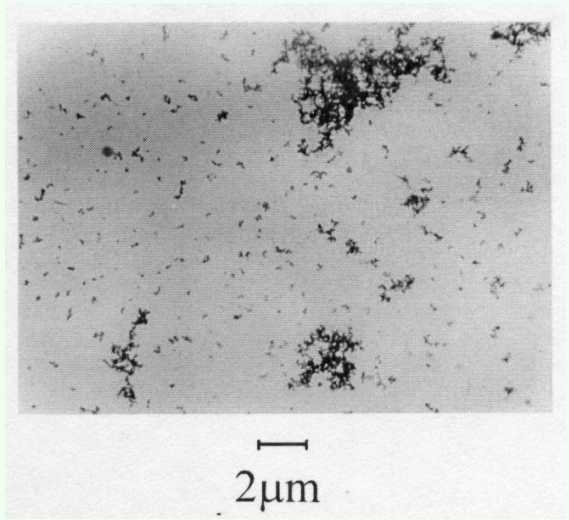
2. Growth kinetics of the self-assembly process: The DLCA model.







Gel



Aerogelation experiment in acetylene diffusion flames
Electron microscope picture inserting a probe into the flame 50ms
(h=4 cm; flow rate: 1.1 cm^3/s)

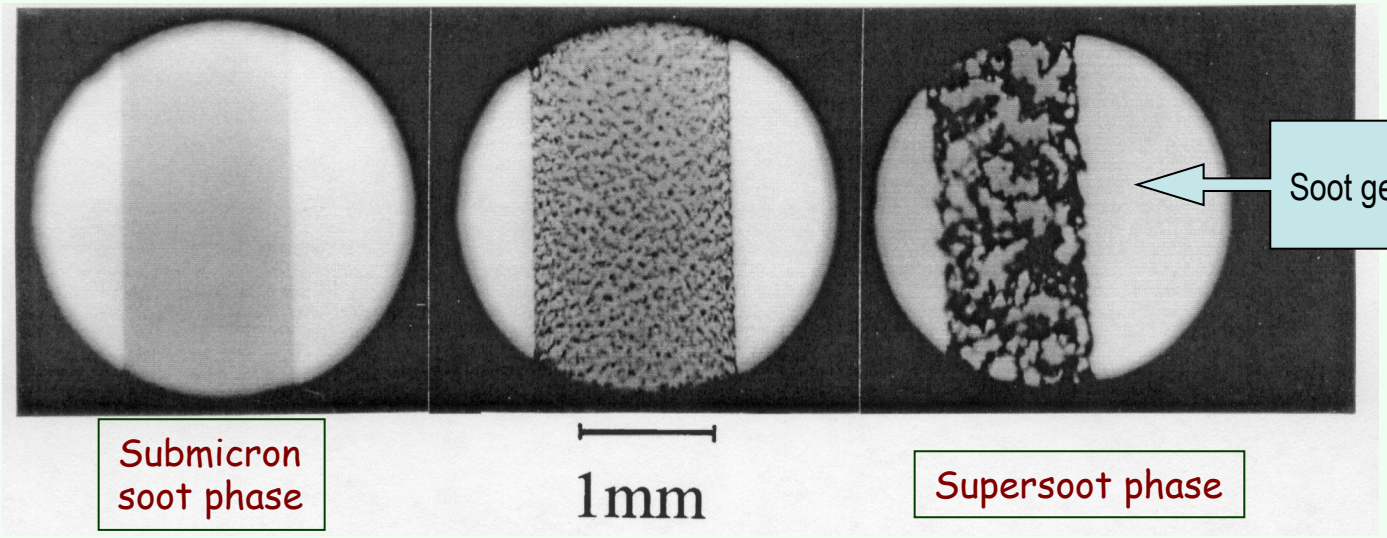
Aerogelation of soot particles in acetylene diffusion flames.

FLAME SOOT **AEROGELATION** experiment C. Sorensen et al., PRL, 80, 1782, (1998)

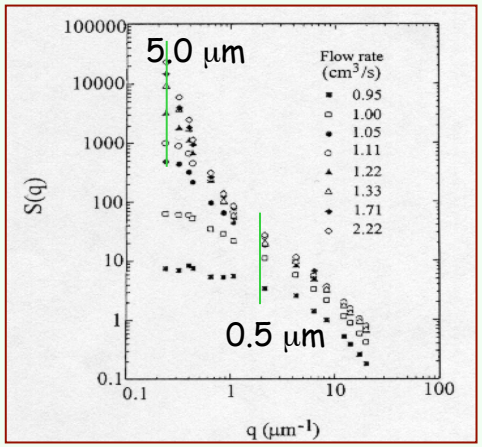
SOOT PARTICLE:

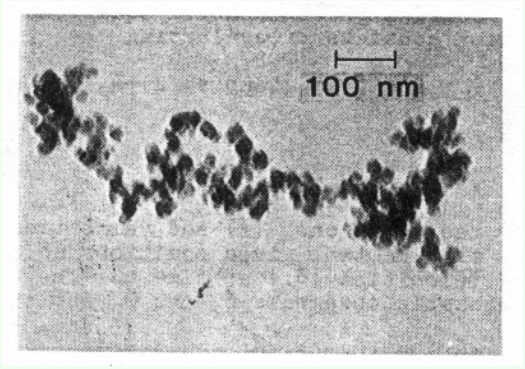
- Carbonaceous soot is a common product of fossil fuel combustion and a major atmospheric pollutant.
- Primary particles are roughly spherical monomers of radii a=10-30 nm.
- Each ramified aggregate has 100's of particles yielding a overall size Rg=50-500 nm.

Flow rate: 0.83 cm^3/s 1.7 cm^3/s 3.4 cm^3/s



OPTICAL STRUCTURE FACTOR (h=10cm)





Fractal aggregates:

$$N = k_0 \left(\frac{R_g}{a} \right)^{D_f}$$

$$D_f \approx 1.8$$

The Mean field Smoluchowski equation.

Case A) An **irreversible** aggregation process:

n_k Number of cluster with k-particles

$$C_k = n_k / V$$

$$\dot{C}_k = \frac{1}{2} \sum_{i+j=k} K_{ij} C_i C_j - C_k \sum_j K_{jk} C_j$$

Moment equations

$$M_n = \sum_i i^n C_i$$

M_0: total number of cluster

M_1: total number of particles

$$\dot{M}_0 = \sum_k \dot{C}_k = \frac{1}{2} \sum_k \sum_{i+j=k} K_{ij} C_i C_j - \sum_k C_k \sum_j K_{jk} C_j = -\frac{1}{2} \sum_{i,j} K_{ij} C_i C_j$$

$$\dot{M}_1 = \sum_k k \dot{C}_k = \frac{1}{2} \sum_k k \sum_{i+j=k} K_{ij} C_i C_j - \sum_k k C_k \sum_j K_{jk} C_j = \sum_i \sum_{j=1}^{i} K_{ij} C_i C_j$$

Mass Conservation: $\dot{M}_1 = 0$

Gel formation: $\dot{M}_1 \neq 0$

In general:

$$\dot{M}_n = \sum_k k^n \dot{C}_k = \ldots = \frac{1}{2} \sum_{i,j} \left[(i+j)^n - i^n - j^n \right] K_{ij} C_i C_j$$

Exact solutions for simple kernels.

1. $K_{i,j} = 1$

$$\dot{M}_0 = -\frac{M_0^2}{2}$$

$$\dot{M}_1 = 0$$

$$\dot{M}_2 = M_1^2$$

$$\dot{M}_3 = 3 M_1 M_2$$

Average particles per cluster: $M_1/M_0 \sim t$

Weight average: $M_2/M_1 \sim t$

Find a generating function: $f(x,t) = \sum_k \left(e^{kx} - 1 \right) C_k(t)$

$$\frac{\partial f}{\partial t} = \frac{1}{2} f^2 \rightarrow f(x,t) = f(x,0) \frac{1}{1 + f(x,0) t/2}$$

For a monodisperse initial condition: $C_k(0) = \delta_{k,1} f(x,0)$

$$C_k(t) = \frac{(t/2)^{k-1}}{(1+t/2)^{k+1}} \sim t^{k-1}$$ for small t

2. $K_{i,j} = i + j$

$$\dot{M}_0 = -M_0 M_1$$
$$\dot{M}_1 = 0$$
$$\dot{M}_2 = 2M_1 M_2$$
$$\dot{M}_3 = 3\left(M_1 M_3 + M_2^2\right)$$

Using the same generating function as before: $f(x,t) = \sum_k \left(e^{kx} - 1\right) C_k(t)$

$$\frac{\partial f}{\partial t} = f\left(\frac{\partial f}{\partial x} - 1\right)$$

For a monodisperse initial condition: $C_k(0) = \delta_{k,1} f(x,0)$

$$u = 1 - e^{-t}$$
$$C_k(t) = (1-u)(ku)^{k-1}\frac{e^{-ku}}{k!}$$

Scott et al. J. Atmosferic Sci. 25, 54 (1968)

3. $K_{i,j} = ij$

$$\dot{M}_0 = -\frac{M_1^2}{2}$$
$$\dot{M}_1 = 0$$
$$\dot{M}_2 = M_2^2$$
$$\dot{M}_3 = 3M_2M_3$$

$$M_2(t) = M_2(0)\frac{1}{1 - M_2(0)t}$$

$$\exists\, t = t_c \;/\; t_c = \frac{1}{M_2(0)t}$$

M_2 and higher moments diverge !!!

GEL formation

Using a generating function: $f(x,t) = \sum_k k e^{kx} C_k(t)$

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x}(f - M_1)$$

$$C_k(t) = t^{k-1}k^{k-2}\frac{e^{-kt}}{k!}$$

In general the reaction kernel K_{ij} must depend on the collision frequency that is related to the relative velocity and cross-section size of the clusters.

- For a fractal object it can be written as:

$$K_{ij} \sim \left(\frac{1}{i} + \frac{1}{j}\right)^{1/2} \left(i^{1/D} + j^{1/D}\right)^{d-1}$$

Relative velocity

Cross-section

Scaling functions

Assume the aggregation kernel is an homogeneous function and λ the degree of homogeneity

$$K_{ai,aj} = a^{\lambda} K_{i,j}$$

Then, the Smoluchowski eq. yields a self preserving scaling function: $C_k = M_1 S_p^{-2} \phi(x)$

Mean cluster size: $S_p = \dfrac{M_p}{M_{p-1}}$

$\phi(x) = A x^{-\lambda} e^{-\alpha x}$ $\qquad x = \dfrac{k}{S_p}$

$\alpha = p - \lambda$

$$M_p(t) = M_p(0) \left(1 + \frac{t}{\tau}\right)^{z(p-1)}$$

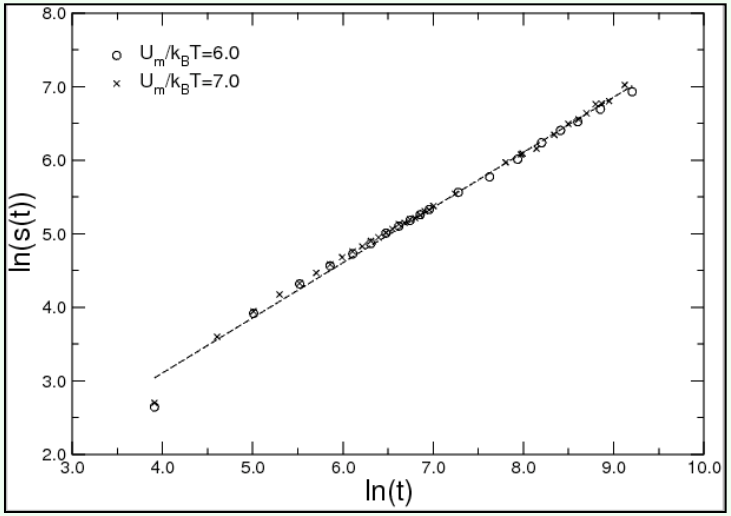
Kinetic exponent: $z = \dfrac{1}{1-\lambda}$

Mean cluster size: $M_0^{-1} \sim t^z$

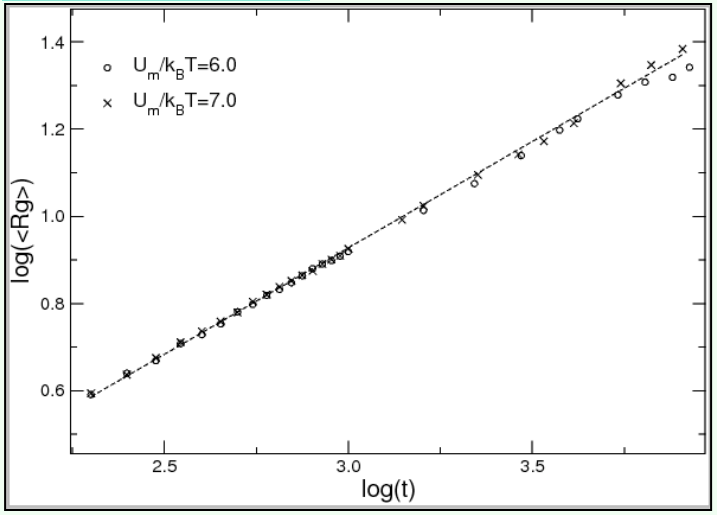
For a Brownian coagulation kernel (in the dilute regime) λ=(d-3)/D

d=3, λ=0, z=1
d=2, λ= -1/D; (D=1.4); z=0.59

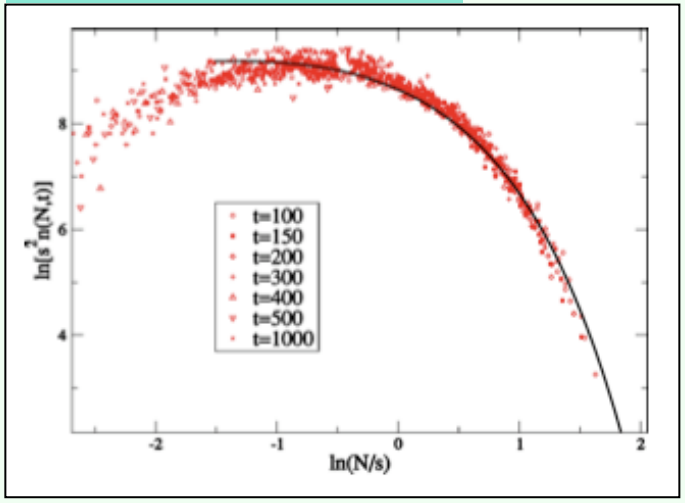
Mean cluster size



$Rg \sim N^{1/D} \sim t^{z/D}$



Test of the scaling ansatz



Case B) A **reversible** aggregation process:

$$A_i + A_j \underset{F_{ij}}{\overset{K_{ij}}{\rightleftarrows}} A_{i+j}$$

$$\dot{C}_k = \frac{1}{2}\sum_{i+j=k}(K_{ij}C_iC_j - F_{ij}C_k) - \sum_j (K_{jk}C_jC_k - F_{jk}C_{j+k})$$

The competition between coagulation and fragmentation leads to a final steady-state configuration characterized by a mean cluster size.

Family et al. PRL, 57, 727 (1986) assumed a steady-state cluster size distribution:

$$C_k(\infty) = M_1 S_p^{-2}\phi(x) \qquad x = \frac{k}{S_p(\infty)}$$

That was further assumed for all times (Sorensen et al. PRL, 59, 363 (1987))

$$C_k(t) = M_1 S_p^{-2}(t)\phi(x) \qquad x = \frac{k}{S_p(t)}$$

In the following we take p=2 for simplicity

Assume both reaction kernels to be homogeneous functions

$$K_{ai,aj} = a^{\lambda} K_{i,j} \qquad K_{i,j} = \kappa_C \Psi_{i,j}$$

$$F_{ai,aj} = a^{\alpha} F_{i,j} \qquad F_{i,j} = \kappa_F \Phi_{i,j}$$

Cluster size: $S(t) = \dfrac{M_2}{M_1}$

$$\dot{S}(t) = \frac{\dot{M}_2}{M_1} \qquad \dot{M}_2(t) = \sum_k k^2 \dot{C}_k$$

$$\dot{S}(t) = A M_1 \kappa_C S(t)^{\lambda} - B \kappa_F S(t)^{\alpha+2}$$

$$A = \int_0^{\infty} dx \int_0^{\infty} dy \; xy \Psi(x,y) \phi(x) \phi(y)$$

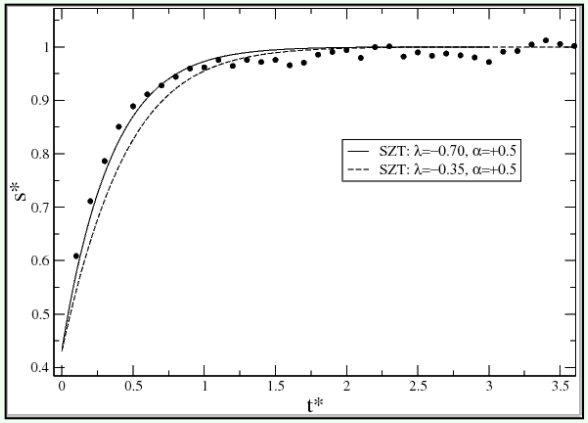
$$B = \int_0^{\infty} dx \int_0^{\infty} dy \; xy \Phi(x,y) \phi(x) \phi(y)$$

Using reduced units:

$$\hat{s} = \frac{S(t)}{S(\infty)} \qquad S(\infty) = \left(\frac{M_1 A \kappa_C}{B \kappa_F} \right)^{\beta}$$

$$\hat{t} = \frac{t}{\tau} \qquad \tau = (M_1 A \kappa_C)^{-(\alpha+1)\beta} (B \kappa_F)^{(\lambda-1)\beta}$$

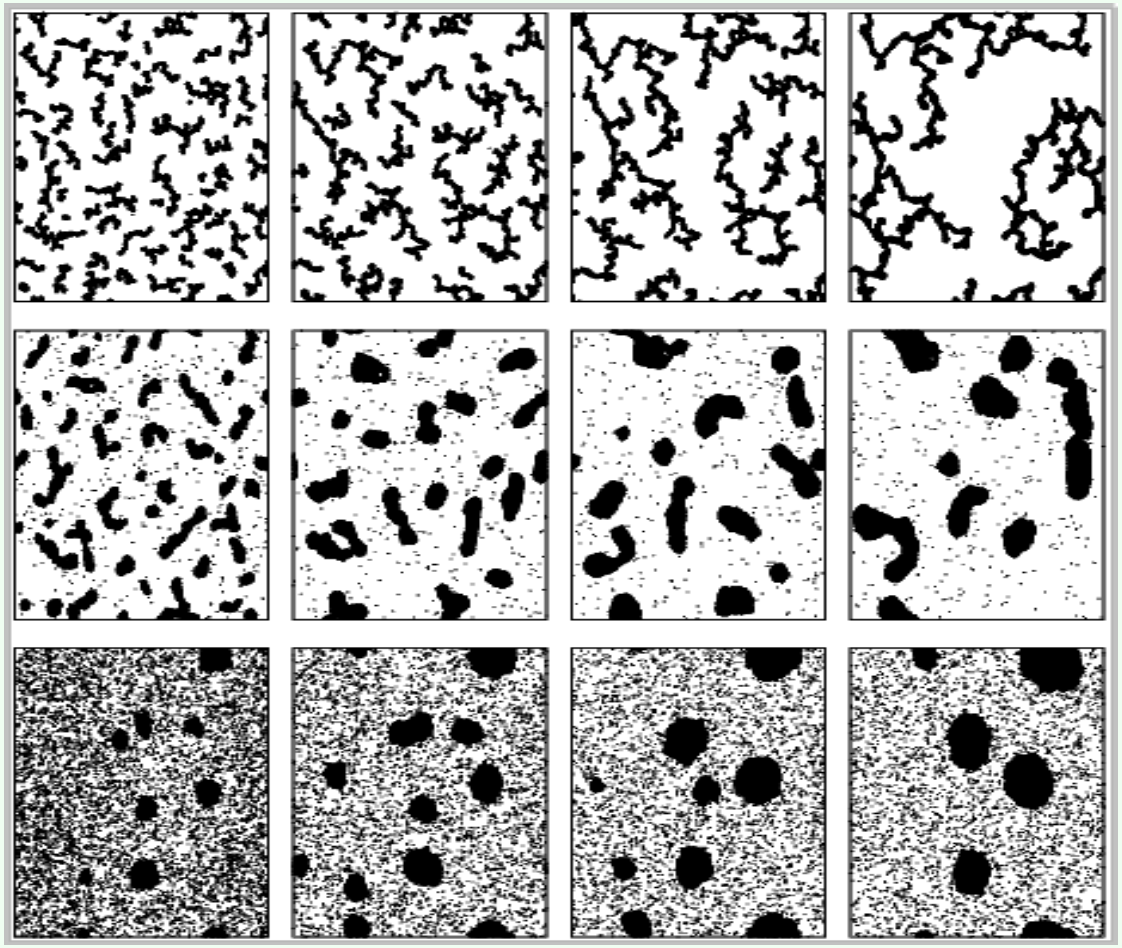
$$\beta = (\alpha - \lambda + 2)^{-1}$$



$$\frac{d\hat{s}}{d\hat{t}} = \hat{s}^{\lambda} - \hat{s}^{\alpha+2}$$

Example: nucleation of colloidal suspensions.
J. Cerdà et al. PHYSICAL REVIEW E **70**, 011405 (2004)

Particles interact via a pair-interaction potential (Asakura-Oosawa)



- # Percolation theory

- Percolation theory is the simplest not exactly solved model displaying a phase transition.

- Let each site in a lattice be occupied at random with probability *p*, that is, each site is occupied (with probability p) or empty (with probability 1−p) independent of the status (empty or occupied) of any of the other sites in the lattice. We call *p* the occupation probability or the concentration.

- A cluster is a group of nearest neighbouring occupied sites.

- The cluster number $n_s(p)$ denotes the number of s-clusters per lattice site.

- The number of clusters of size s in a hypercubic lattice of linear size L is $L^d n_s(p)$, d being the dimensionality of the lattice.

- For a finite lattice $L < \infty$ if the occupation probability is small there is a tiny chance of having a cluster percolating between two opposite boundaries, whereas for $p \to 1$ we almost certainly find a cluster percolating through the system.

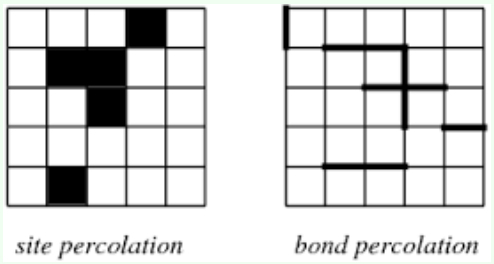
- The percolation threshold p_c is the concentration (occupation probability) p at which an infinite cluster appears for the first time in an infinite lattice.

- In a finite system p_c depends on the lattice shape, connectivity (site/bond) and dimensionality.

The aim of the percolation theory is to characterize the number and properties of the clusters formed

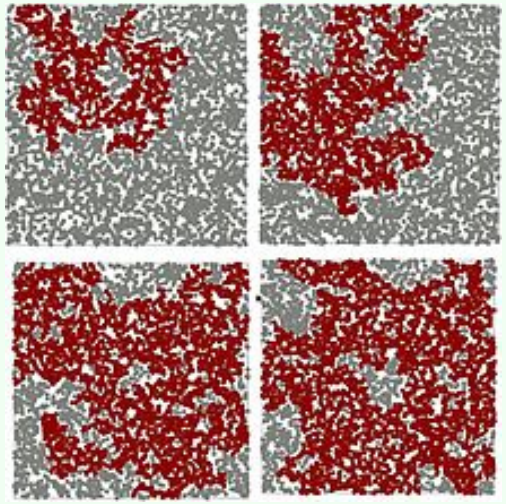
Occupied and empty sites can represent different physical properties

Occupied	Empty
conductor	isolator
magnet	paramagnet
working computer	damaged computer



And has a large number of applications, such as:

- Epidemics.
- Fire spreading.
- Oil recovery from amorphous and porous material.
- Sol-gel transition.
- Polymerization.
- […]



Examples of p_c values for different systems:

	d=1	d=2		d=3
Lattice	line	triangular	square	cubic
P_c	1	0.5	0.5927	0.3116

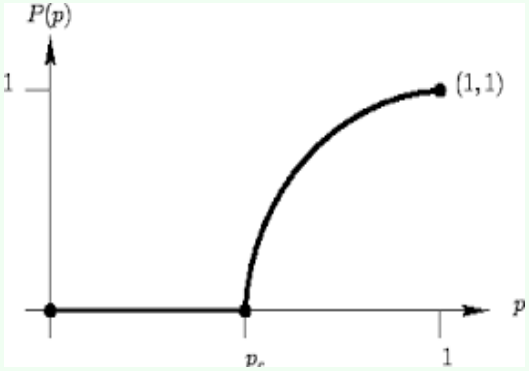
Critical behavior

In analogy with the magnetic phase transition (*p* plays the role of the temperature):

- $p<p_c$ disordered phase
- $p>p_c$ orderered phase

(2d) Ising model:

- Magnetization: $M \sim (T - T_c)^{\beta=1/8}$
- Magnetic susceptibility: $\chi \sim |T - T_c|^{-\gamma=-4/3}$
- Correlation length: $\xi \sim |T - T_c|^{-\nu=-1}$



Percolation:

- Prob. a lattice site belongs to an infinite cluster: $P_\infty \sim (p - p_c)^\beta$
- Average size of finite clusters: $s \sim |p - p_c|^{-\gamma}$
- Average distance between 2 sites in the same cluster: $\xi \sim |p - p_c|^{-\nu}$

(2d-square latttice) $\beta = 5/36;\ \gamma = 43/18;\ \nu = 4/3$

Exact solution in 1d

Prob that a lattice of size L percolates at a probability p: $\Pi(p, L)$

$$\lim_{L\to\infty} \Pi(p, L) = \begin{cases} 0 \text{ if } p<p_c \\ 1 \text{ If } p>= p_c \end{cases}$$

$$\Pi(p, L) = p^L \qquad \lim_{L\to\infty} p^L = \begin{cases} 0 \text{ if } p<p_c \\ 1 \text{ If } p>= p_c \end{cases} \qquad \Longrightarrow \qquad p_c = 1$$

Cluster or size s (per unit volume): $n_s(p)$

$$\begin{aligned} n_s(p) &= (1-p)p^s(1-p) = (1-p)^2 p^s \\ &= (1-p)^2 \exp\left[\ln p^s\right] = (1-p)^2 \exp\left[s \ln p\right] = (1-p)^2 \exp\left[-s/\xi\right] \end{aligned}$$

$\xi = -\dfrac{1}{\ln p}$ is the characteristic cluster size

$$n_s(p) = (p_c - p)^2 \exp\left(-s/\xi\right)$$

$$\xi = -\frac{1}{\ln p} = -\frac{1}{\ln\left[p_c - (p_c - p)\right]} \to \frac{1}{P_c - p} = (p_c - p)^{-1} \qquad \nu = 1$$

Occupied sites (per unit volume): $\sum_s s n_s(p) = p$

Probability that an occupied site belongs to a cluster of size s: $\omega_s = \frac{s n_s(p)}{\sum_s s n_s(p)}$

Mean cluster size: $S(p) = \sum_s s\omega_s = \ldots = \frac{1+p}{1-p} \quad \to \frac{p_c+p}{p_c-p}$

$$\lim_{p\to p_c} S(p) = \lim_{p\to p_c} \frac{p_c+p}{p_c-p} \to \frac{2p_c}{p_c-p} \sim (p_c-p)^{-1} \qquad \gamma = 1$$

Funrther reading:
Introduction To Percolation Theory. Dietrich Stauffer, Ammon Aharony

Animations in the web

https://en.wikipedia.org/wiki/Forest-fire_model
https://www.youtube.com/watch?v=2hmmcl0kd5M
https://www.youtube.com/watch?v=bUd4d8BDIzI

• Surface growth and the KPZ equation.

- The structure of many systems can be described in terms of more or less uniform and continuous homogeneous regions separated by (disordered) interfaces at which physical or chemical properties change abruptly.

- Such interfaces often cannot be adequately described in terms of simple euclidean shapes and appear to exhibit self-affine scaling. Fractal geometry and scaling laws, allow us to study the processes taking place near such random rough surfaces as well as the nature of the interface itself.

- Applications in:
  - Electrochemical deposition
  - Corrosion and oxidation
  - Fluid-fluid displacement
  - Growth of cell colonies
  - Thin film and epitaxial growth (ballistic deposition models)

Growth process:

Propagation of a front (active zone) leading behing a (frozen) structure that provides a record of its passage.

Characterization of rough surfaces:

- $\xi_\perp$ Perpendicular correlation length (width of the surface –active zone-)
- $\xi_\parallel$ Parallel correlation length (lateral distance over which surface heigth fluctuations are correlated).

$$\xi_\perp = \left\langle |h_i - \bar{h}|^q \right\rangle^{1/q} \sim t^\beta$$

$$\xi_\parallel \sim t^{1/z}$$

Heigh difference correlation: $C_q(\vec{x}) = \langle |h(\vec{x} - \vec{x}_0) - h(\vec{x}_0)|^q \rangle^{1/q}$

$$C_q(x) = \langle C_q(\vec{x}) \rangle_{|\vec{x}|=x}$$

$$C_q(x) = x^{H_q} \mathcal{F}_q(x/\xi_\parallel)$$

$$\mathcal{F}_q(y) = \begin{cases} C, & y \ll 1; \\ y^{-H_q}, & y \gg 1 \end{cases} \qquad C_q(x) \sim \begin{cases} x^{H_q}, & x \ll \xi_\parallel; \\ \xi_\parallel^{H_q}, & x \gg \xi_\parallel \end{cases}$$

$$\xi_\perp = C_q(x \gg \xi_\parallel) \sim \xi_\parallel^{H_q}$$

In many cases: $H_q = H = \alpha$ $\qquad \xi_\parallel \sim \xi_\perp^{1/\alpha}$ $\qquad \boxed{z = \dfrac{\alpha}{\beta}}$

Kinetic exponent: z
Roughness exponent: α

Different sets of exponents lead to different universality classes

Basic equations:

1. The growth of the surface is driven by a random proces (deposition of particles onto a cold surface).

$$\frac{\partial h(\vec{x},t)}{\partial t} = \eta(\vec{x},t)$$

$$\langle \eta(\vec{x},t) \rangle = 0$$

$$\left\langle \eta(\vec{x},t)\eta(\vec{x'},t') \right\rangle = 2\mathcal{D}\delta(\vec{x}-\vec{x'})\delta(t-t')$$

$$\beta = \frac{1}{2}$$

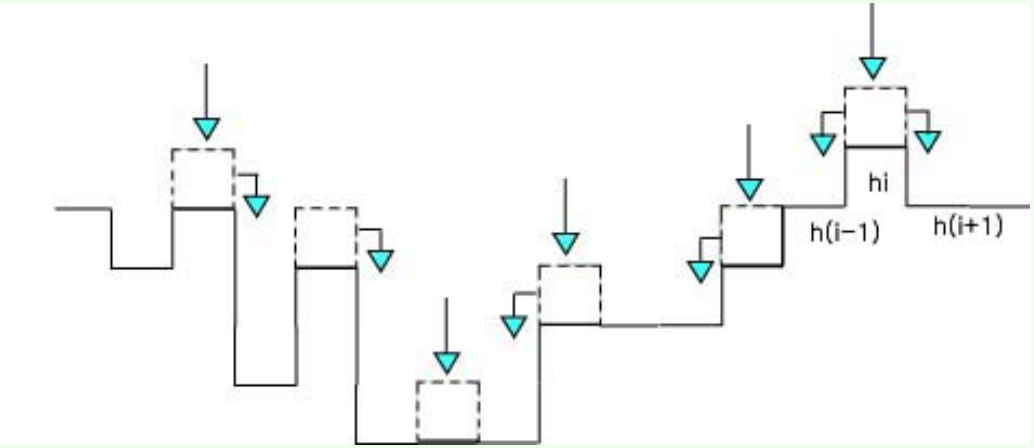
In a numerical model, column (i) is selected at random and is increased 1 unit.

$$h_i' = h_i + 1$$

2. Random deposition with surface relaxation. The EDWARDS- WILKINSON (EW) model.
Proc. Royal Society A, 381, 17 (1982)

Assume a weak flux of particles along the steepest descent path onto the surface.

$$\frac{\partial h(\vec{x},t)}{\partial t} = a\nabla_d^2 h(\vec{x},t) + \eta(\vec{x},t)$$



Schematic representation of its numerical implementation.

- Column (i) is selected at random.
- A new particle added to this column remains in this position if:

$$h_i \leq min(h_{i-1}, h_{i+1})$$

- Otherwise diffuses to the lowest nearest neighbour column.

- Exponents in 1+1 dimension.

  Assuming the growth process is invariant under the transformation:

$$\begin{cases} x \to \lambda x \\ h \to \lambda^{\alpha} h \\ t \to \lambda^{z} t \end{cases}$$

$$\lambda^{\alpha - z} \frac{\partial h(\vec{x}, t)}{\partial t} = a\lambda^{\alpha - 2} \nabla_d^2 h(\vec{x}, t) + \lambda^{-(d+z)/2} \eta(\vec{x}, t)$$

  Dimensional analysis:

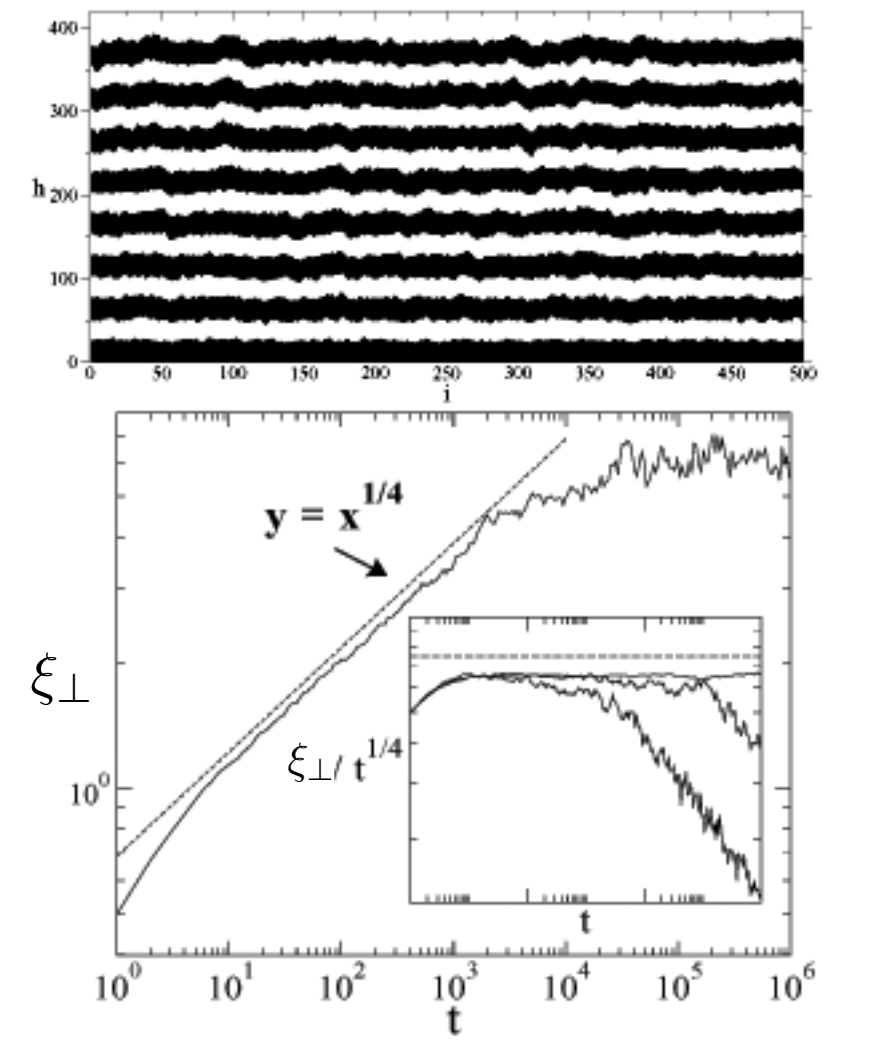
$$\alpha - z = \alpha - 2 = -(d + z)/2$$

$$\begin{cases} z = 2 \\ \alpha = \frac{2-d}{2} = \frac{1}{2} \\ \beta = \frac{\alpha}{z} = \frac{1}{4} \end{cases}$$

- In 2+1 dimension.

  Since the EW is a linear equation. A FT provides the amplitudes of the evolving surface

$$\xi_{\perp} \sim \begin{cases} [\log(t)]^{1/2} & \text{at short times;} \\ [\log(L)]^{1/2} & \text{at long times.} \end{cases}$$



L=500 (=time unit: tu)
After 50 tu change color

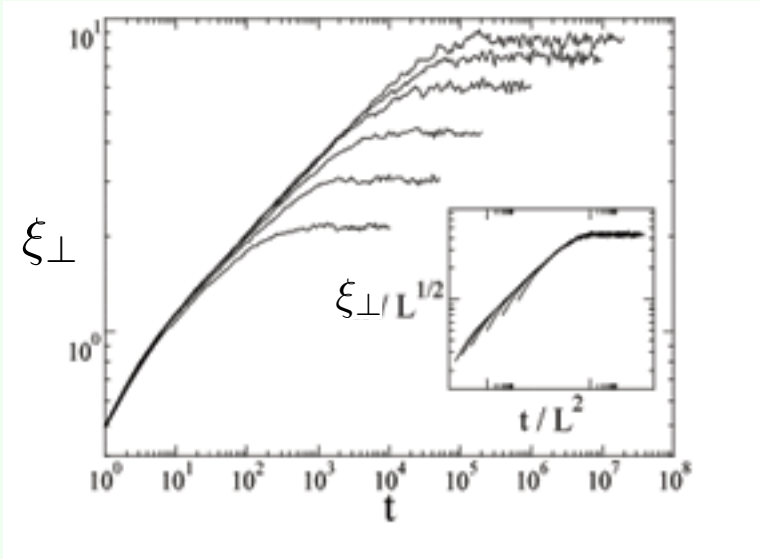
FINITE SIZE EFFECTS

$$\xi_{\|} \sim t^{1/z}$$

Due to finite system size: $\xi_{\|} \sim L \quad t_c \sim L^z$

$$\xi_{\perp} \sim \xi_{\|}^{\alpha} \sim L^{\alpha}$$

$$\boxed{\xi_{\perp}/L^{\alpha} = \mathcal{F}(t/L^{z})}$$



Roughness against time for different system sizes.
Data collapse is obtained for α=1/2 and z=2

3 Ballistic deposition. The KPZ equation.

Phys. Rev. Lett, , 56, 889 (1986)

Was originally proposed as a simple model for sedimentation, and it is closely related to stirred fluids (turbulence) and directed polymers in random media.

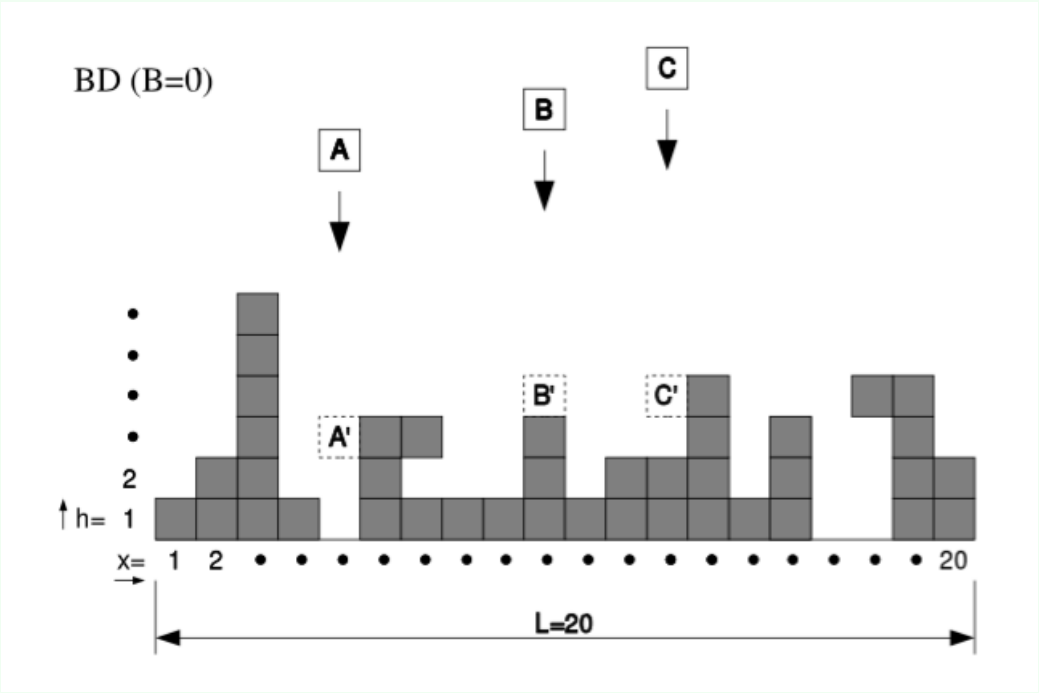
Takes into account the growth that occurs at local normals to the surface. (EW eq. does not)

By using RG techniques, it has been conjectured that the KPZ equation is the field theory of many surface growth models, such as the Eden model, ballistic deposition and the SOS model.

$$\frac{\partial h(\vec{x},t)}{\partial t} = a\nabla^2 h(\vec{x},t) + b\left(\nabla h(\vec{x},t)\right)^2 + \eta(\vec{x},t)$$

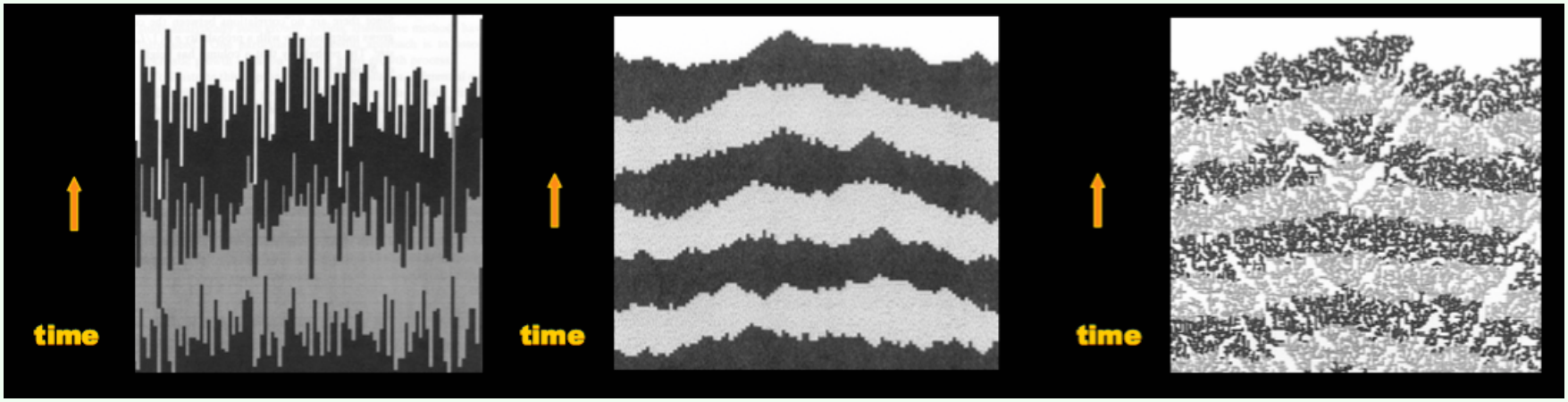
Due to the non-linear term, exponents cannot be derived from scale invariance !

- 1+1 dim: $\alpha = \frac{1}{2}, \quad \beta = \frac{1}{3}$
- 2+1 dim: $\alpha \approx \frac{2}{5}, \quad \beta \approx \frac{1}{4} \qquad \frac{1}{z} > \frac{1}{2}, \quad \xi_{\parallel}$ Is superdiffusive



Case A $$h'_i = max(h_{i-1}, h_i + 1, h_{i+1})$$

Case B $$\begin{cases} h'_{i-1} = max(h_{i-1}, h_i) \\ h'_i = h_i + 1 \\ h'_{i+1} = max(h_{i+1}, h_i) \end{cases}$$



random EW BD

See animations from:
https://www.youtube.com/watch?v=zYhqh8dvTUs

- # Collective behavior: Flocking, swarming and herding.

① Collective behavior shown in birds, fish, bacteria, insects, … humans, that arises from simple rules that are followed by the individuals and does not involve any central coordination.

② Rules:

i. Separation (short-range repulsion)
ii. Alignment (Steer towards the average heading of the neighbours)
iii. Cohesion (long-range attraction)

③ Models:

Novel Type of Phase Transition in a System of Self-Driven Particles. T. Vicsek, et al. PRL, 75, 1226 (1995).

Point-like particles. No collective motion is possible in the zero-density limit case.

Onset of Collective and Cohesive Motion. Guillaume Gregoire and Hugues Chate, PRL, 92, 025702 (2004).

Adds a LJ interaction term.

$$\vec{x}_i(t+1) = \vec{x}_i(t) + \vec{v}_i(t)\Delta t$$

$$\vec{v}_i(t+1) = |\vec{v}|(\cos\theta(t+1), \sin\theta(t+1))$$

$$\theta(t+1) = \arctan\left(\frac{\langle \sin\theta(t)\rangle_r}{\langle \cos\theta(t)\rangle_r}\right) + \Delta\theta$$

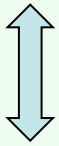
$$\begin{cases} \Delta t = 1 \\ r = 1 \text{ interaction radius} \\ \Delta\theta \in [-\eta/2, \eta/2] \text{ noise} \\ \rho = N/L^d \text{ particle density} \end{cases}$$

Order parameter

$$v = \frac{1}{N|\vec{v}|}\left|\sum_{i=1}^{N}\vec{v}_i\right|$$

Phase transition:

Random motion with small correlations $\rho\,\eta$



Ordered motion $\rho\ \eta$

$$v \sim [\eta_c(\rho) - \eta]^{\beta}$$

$$v \sim [\rho - \rho_c(\eta)]^{\delta}$$