Model of Diffusion—Diffusion Limited Aggregation

Phys349B
Hamiltonian mechanics

Gretchen C. Apr/2004

1-D diffusion

- Random walk behaviour
- Diffusive equation:

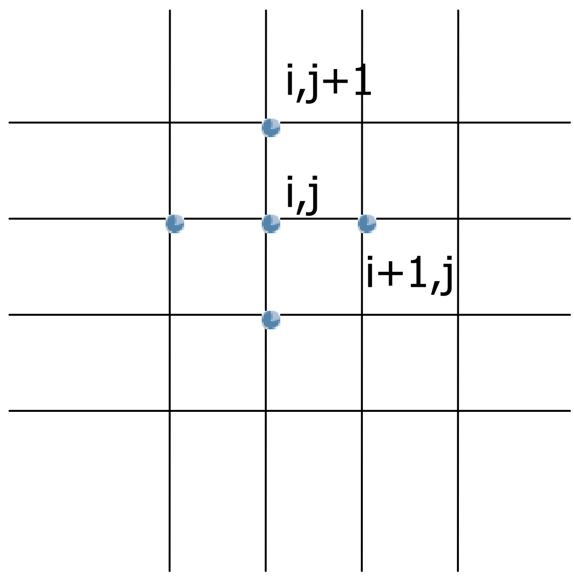
$$\frac{\partial u(x,t)}{\partial t} = \eta \nabla^2 u(x,t)$$

u(x,t): density

η : diffusion constant

- Deterministic: given initial density u(x, 0), future profile u(x, t) can be predicted by solving the ODE equation.

Diffusion in a lattice



Lattice spacing=a

$$\frac{\partial u}{\partial x} = \frac{u_{i+1,j,t} - u_{i,j,t}}{a}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j,t} - 2u_{i,j,t} + u_{i-1,j,t}}{a^2}$$

Diffusion Limited Aggregation (DLA)

- Limited – a seed particle is placed at the center and cannot move

- Aggregation – a second particle is added randomly at a position away from the center. It sticks with the first particle or diffuses out the lattice. The process is repeated several times.

- A circle drawn to enclose the cluster -> Rmin (note, the particle is added outside Rmin)

DLA = a fractal structure

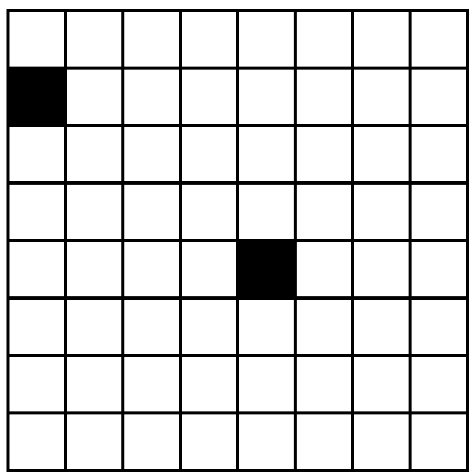
- DLA has a fractal structure and the fractal dimension can be calculated by:

$$D = \frac{\ln N}{\ln R_{\min}}$$

N: number of particles

- Why a fractal structure??

DLA (con't)

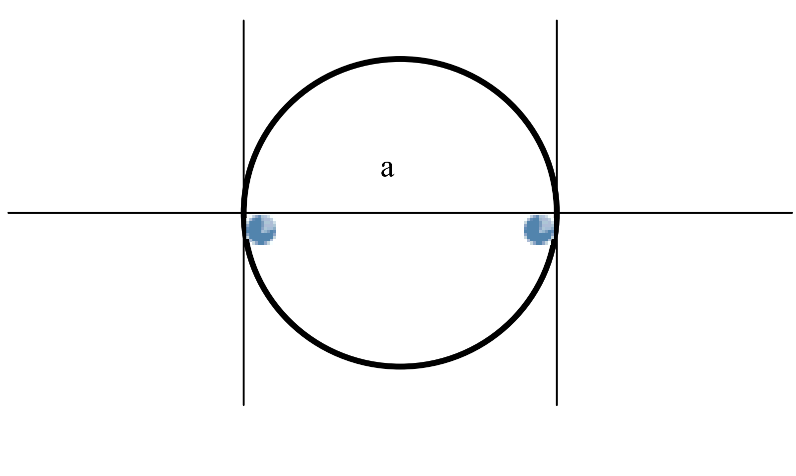


A primitive DLA model

Very slow~~ but I'm not intending to waste time here

DLA (con't)

- 2^{nd} particle sticks with the seed particle at any of the four neighbours (if it didn't leave the lattice)
- A circle drawn to enclose the two particles.
- radius = Rmin = a/2



DLA (con't)

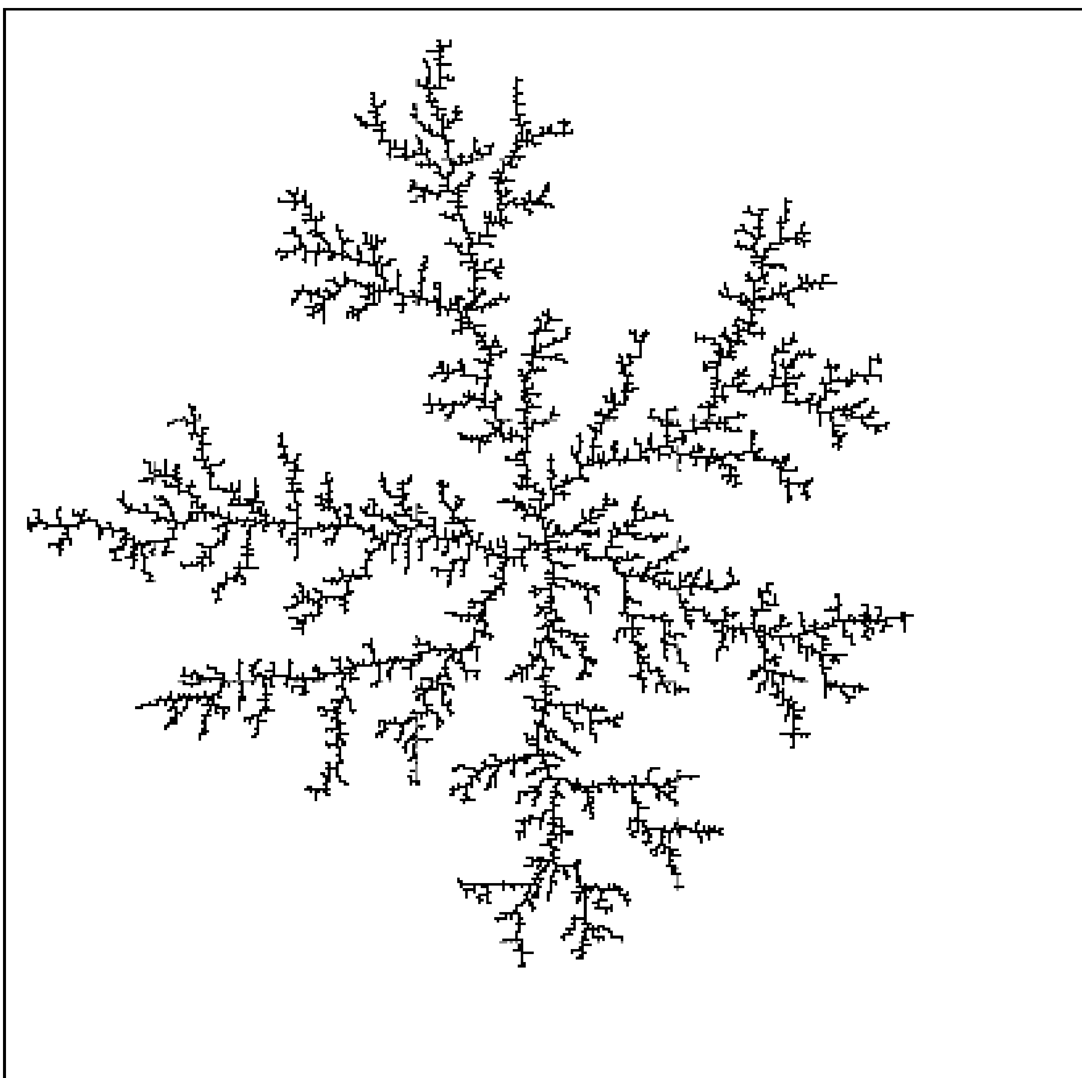
- Add many many particles, and increase Rmin to enclose the whole cluster.

- Run a simple Mathematica program to see how it happened.

- We can get something quite impressive. (if you have extraordinary computer simulation programming skills that is).

DLA (con’t)

Sticking Coefficient $\xi = 1.$



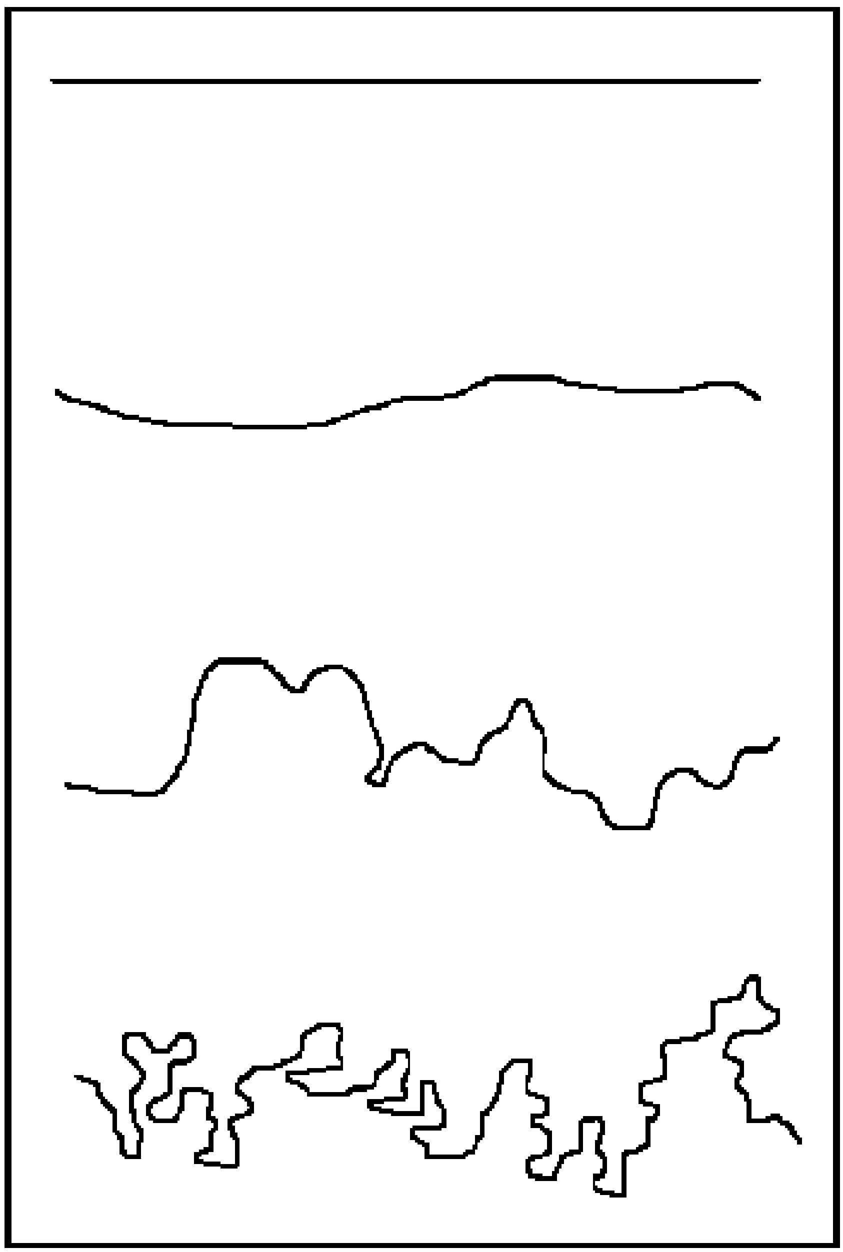
Fractal

- a set with fractional dimension

- such as the BC coastline, which has a fractal dimension $1<D<2$

- A line has $D=1$, a plane $D=2$

- Most of the well known fractal structures have self-similarity property – an enlargement of a section of the fractal resembles the original fractal structure

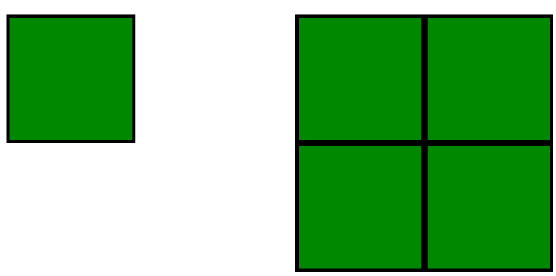


Topologische Dimension	Fraktale Dimension
1	1.00
1	1.02
1	1.15
1	1.35

Fractal (con't)

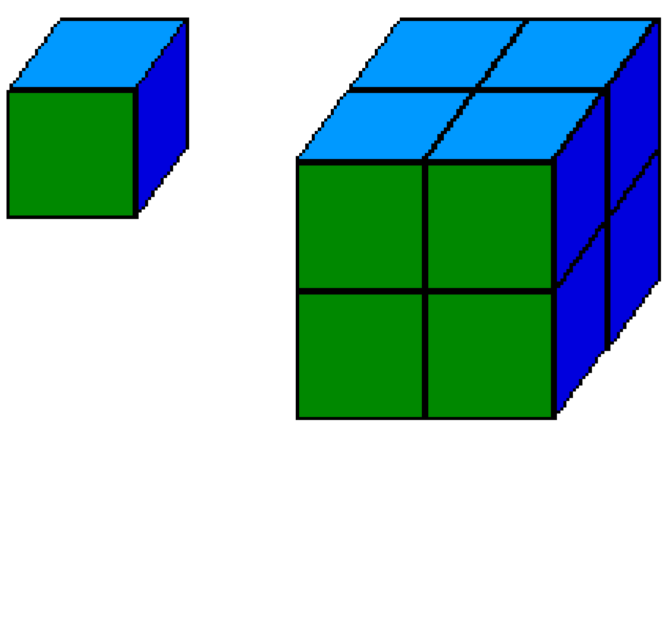
Double the size, double the mass.

$M = k \cdot L^1$



Double the size, quadruple the mass.

$M = k \cdot L^2$



Double the size, multiply the mass by 8.

$M = k \cdot L^3$

Fractal (con't)

- Amount of mass of an object inside a circle of radius r has a power law relation:

$$M(r) = kr^D$$

Where D is a fractal dimension.

Therefore…

- Denote the number of particles as N(R) which is closer than some distance R away:

$$N(R) = kR^{D}$$

- To calculate the fractal dimension, take the logarithm both sides:

$$D = \frac{\ln(N)}{\ln(R)}$$

- Log-log plot of N and R gives us the slope = D, the fractal dimension

Anyway, back to my very primitive DLA model…

- Using the equation to calculate the fractal dimension gives…

… something between 1 and 2, which is reasonable.

- Shrink spacing ‘a’, and using the lattice constant instead of Rmin…

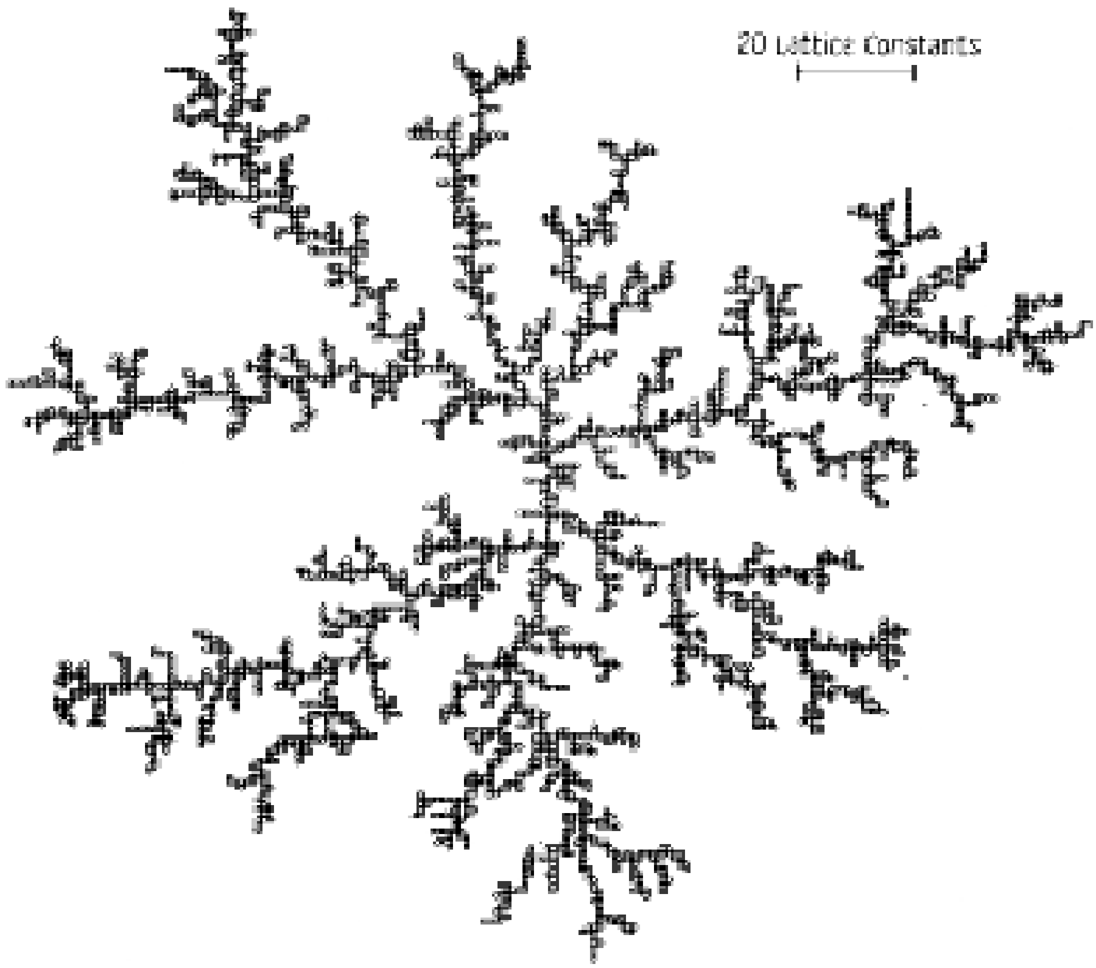


FIG. 1. Random aggregate of 3600 particles on a square lattice.

- 3600 particles aggregation
- radius ~ 85 lattice constant
- D ~ ln(3600)/ln(85)~1.87

Original method

- By computing density correlation function:

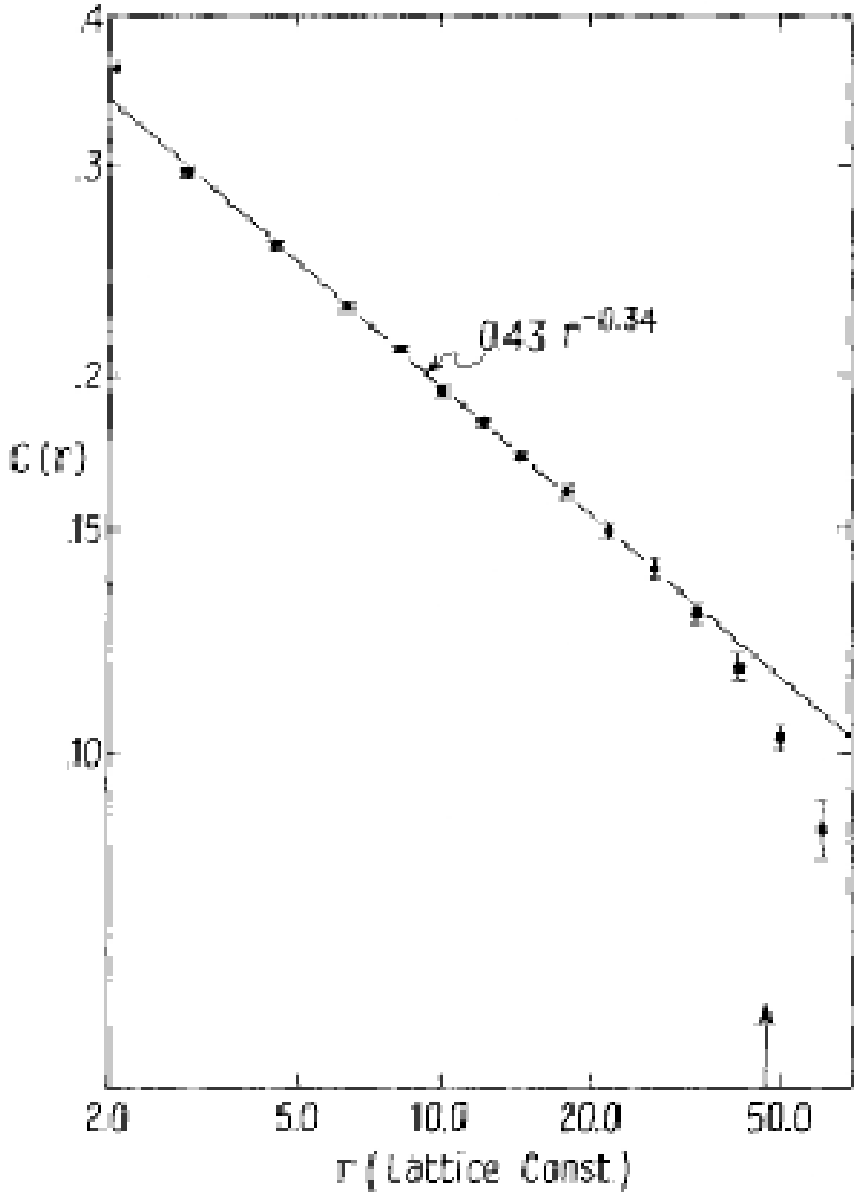
$$C_T(r) = < \rho(r')\rho(r' + r) >$$

- density correlation function for N-particle aggregation gives information about particle distribution:

$$C(r) = N^{-1}\sum_{r'}\rho(r')\rho(r' + r)$$

C(r): average density
r: distance separating the two sites

(this is an approximation to the ensemble average correlation function-> works for r << R)



Plot of C(r) vs. r

- C(r) averaged over directions and over six aggregates of ~3000 particles
- result: $C(r) \sim r^{-0.34}$

Fractal dimension again…

- C(r) can be considered as a measurement of the density in a shell with mass dM(r), radius r and thickness dr:

$$C(r) = \frac{dM(r)}{2\pi r dr}$$

We know that $M(r) \sim r^D$

Therefore,

$$C(r) \sim \frac{r^{D-1}dr}{2\pi r dr} \sim r^{D-2} \equiv r^{D-d}$$

D obtained

Experimental result also gives:

$$C(r) \sim r^{-\alpha} \equiv r^{-0.34}$$

The fractal dimension can be calculated:

$$D = -\alpha + d$$

d: Euclidean dimension
D: fractal dimension

D ~ -0.34 + 2 = 1.66
…. is the fractal dimension obtained.

Why a fractal??

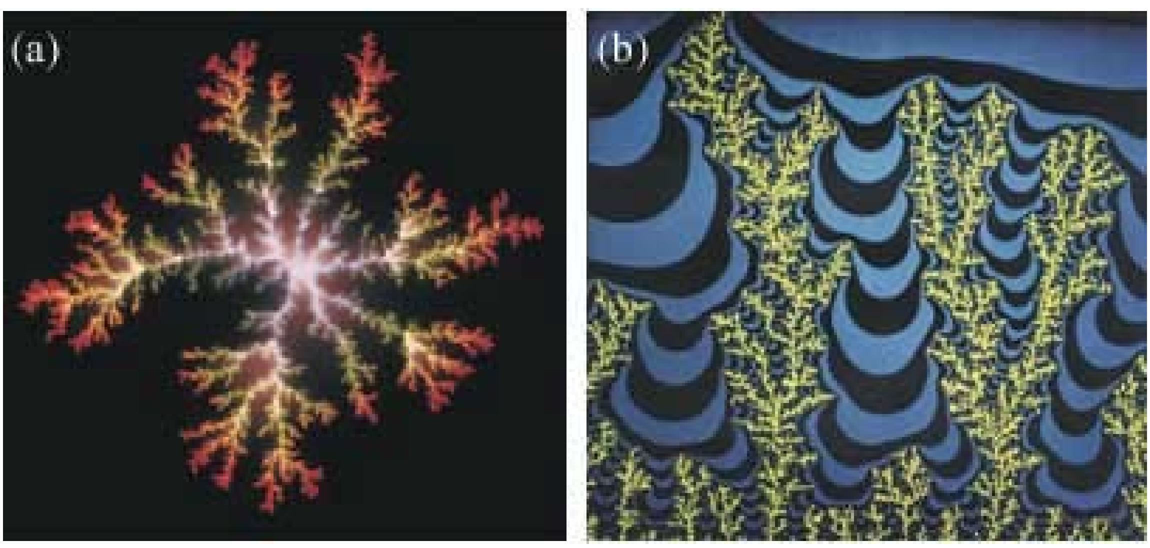
• DLA is obviously a self-similar fractal structure

• the particles are more likely to stick to the tips of the branches.

• difficult for the particles to penetrate deeply into the valleys without first contacting any surface site -- the tips 'screens' the fjords

• observed with a density probability equipotential graph…

Cool pictures from Physics Today



(b) is the density probability equipotential graph

A quick mention of sticking coefficient

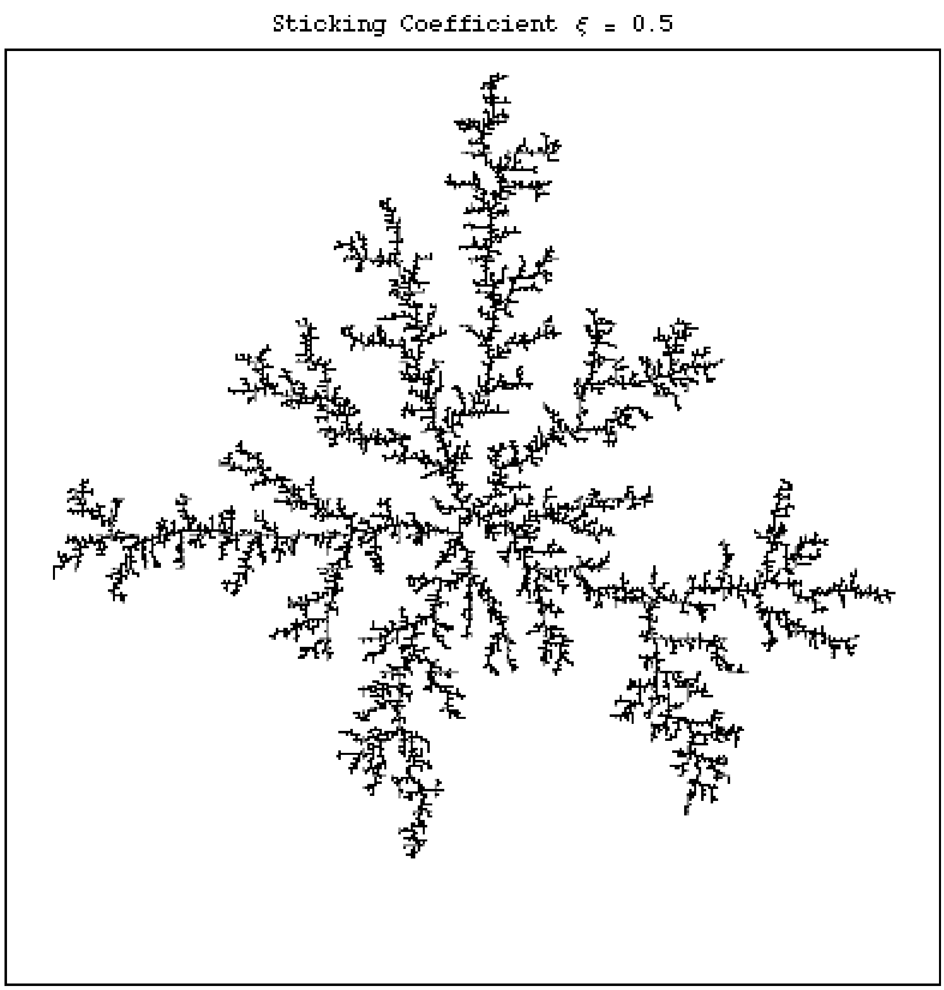
- We can introduce a sticking coefficient in the computer simulation program for a DLA model

- Sticking coefficient is the probability the particle with stick to the cluster.

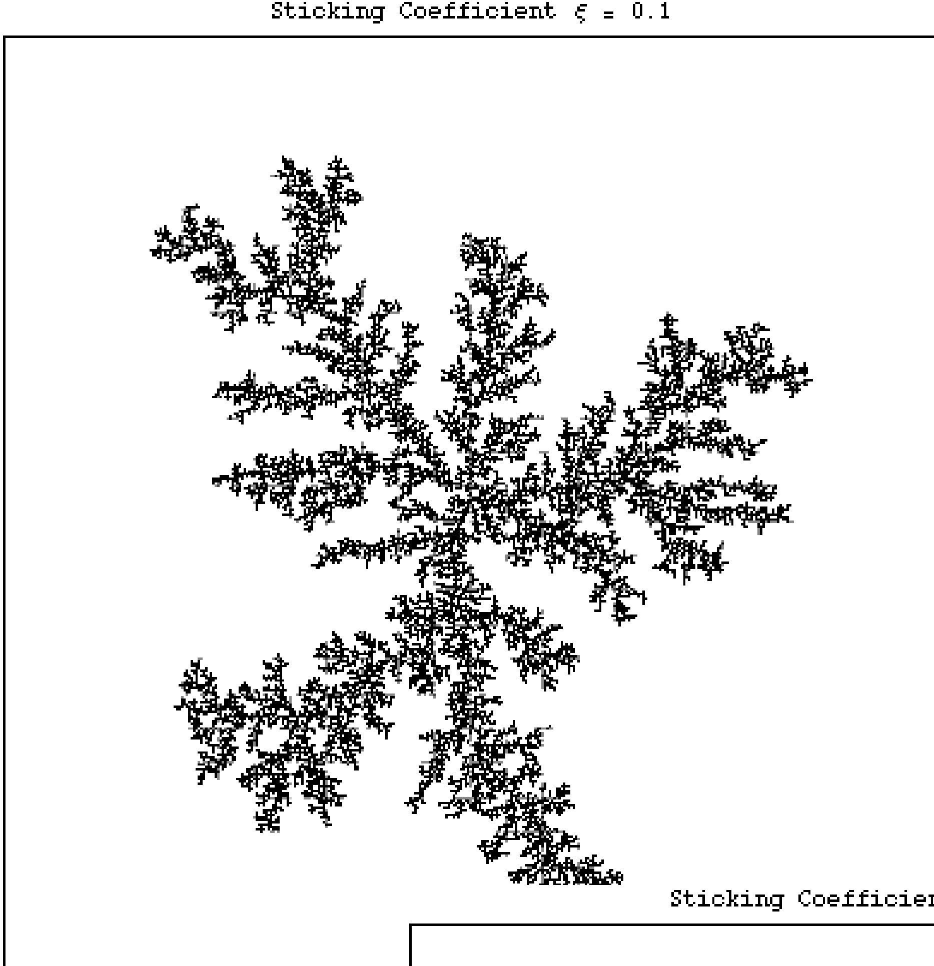
- With low sticking coefficient, a particle will tend to move along the occupied sites until eventually sticks

- Previous calculation was obtained with sticking coefficient set to one -- the particle sticks right after it is at the neighbourhood of another particle.

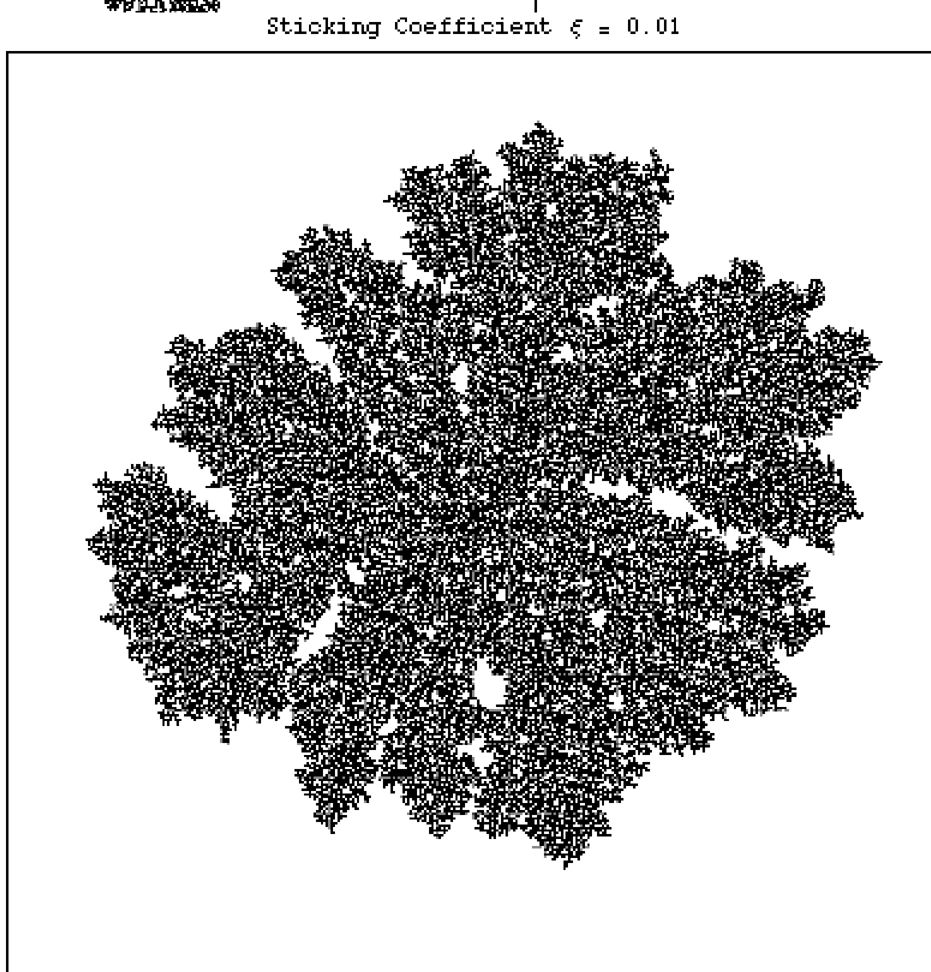
DLA model with different sticking coefficient



S.C.=0.5



S.C.=0.1



S.C.=0.01

Acknowledgement

Hope I didn't miss anything….

Phew… it's finally done~

Despite the amount of brain cell-killing thinking process, this is still my favourite course of the year.
So thanks to….

Mona
Ryan M (so I actually finished it on time)
Jordan
And.. Everybody else in the class
Also….

Give credits where credits are due…

The original author of the DLA model:

T.A. Witten
L.M. Sander

Well, that should be more than 20 minutes…

If not, here's a weird animation my godbrother, Tony, made: