DLA Simulations

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Aim

- To Use Monte-Carlo Method (Random Walkers)/DLA to simulate growth pattern of an air bubble expanding in a Newtonian fluid.
- To understand how the simulation can be applied to other processes.

Outline

- Background Information:Dimensions and Fractals
- Theoretical Treatment
- Numerical Simulation, by a not so obvious process, and the details of the experiment
- Why the Numerical Simulation (DLA) actually does represent the expanding air bubble
- Conclusion: Fractal Nature of DLA and resulting applications

Dimensions

- The dimension/dimensionality of an object is a topological measure of the size of its covering properties. Roughly speaking, it is the number of coordinates needed to specify a point on the object.

Lebesgue covering dimension

- Dimensions can be defined in varying number of ways. One such dimension is the **Lebesgue covering dimension**- also known simply as the topological dimension. It is defined in terms of covering sets, and is therefore also called the covering dimension.
- Cover: A family g of nonempty subsets of *X* whose union contains the given set *X* (and which contains no duplicated subsets) is called a cover (or covering) of *X*. For example, there is only a single cover of {1}, namely {1} itself. However, there are five covers of {1,2}, namely {{1}, {2}}, {{1,2}}, {{1},{1,2}}, {{2},{1,2}}, and {{1},{2},{1,2}}. The basic idea here is that dimension can vary depending on the covering sets.

Lebesgue …. Contd.

- There are several branchings and extensions of the notion of topological dimension. Implicit in the notion of the Lebesgue covering dimension is that dimension, in a sense, is a measure of how an object fills space. If it takes up a lot of room, it is higher dimensional, and if it takes up less room, it is lower dimensional.

- Hausdorff dimension (also called fractal dimension) is a fine-tuning of this definition that allows notions of objects with dimensions other than integers. Fractals are objects whose Hausdorff dimension is different from their topological dimension

Fractals

- A fractal is an object or quantity that displays ***self-similarity***. The object need not exhibit *exactly* the same structure at all scales, but the same "type" of structures must appear on all scales.

- Examples:

Fractal Dimension

The *fractal dimension* is the basic notion for describing structures that have such scaling symmetry. To provide for a measure for filling space, we have the ***D***-dimensional *Hausdorff measure* on a set ***S***

$$M_D(S) = \lim_{\varepsilon \to 0} \inf_{r_k < \varepsilon} \sum_k r_k^D,$$

(***D > 0,*** real) This defines the optimal covering of this set using spheres of variable radius r_k. The value of ***D*** at which M_D jumps from Infinity to ***0*** is defined as the *Hausdorff-dimension* D_H .

Box-dimension

The *capacity-dimension* $\boldsymbol{D_C}$, defines a partition of the fractal into *equally sized* cubes with edge size ε

$$D_C = \lim_{\varepsilon \to 0} \frac{\ln N(\varepsilon)}{\ln 1/\varepsilon}.$$

$N(\varepsilon)$ denotes the minimum number of cubes required for covering the set. (This is also the technique used by the software we have used to calculate the fractal dimensions of the objects)

Theoretical Treatment

- The velocity of water in the Hele Shaw cell is given by:

  $$v= -b^2 \nabla p/ 12 m$$

  where b= gap between the 2 glass pieces, and m is fluid viscosity.
- Also, assuming that fluids are incompressible $\nabla v=0$, and hence

  $$\nabla^2 p=0$$
- This establishes that Laplace equation is satisfied. Also, the pressure difference between air and water is given by

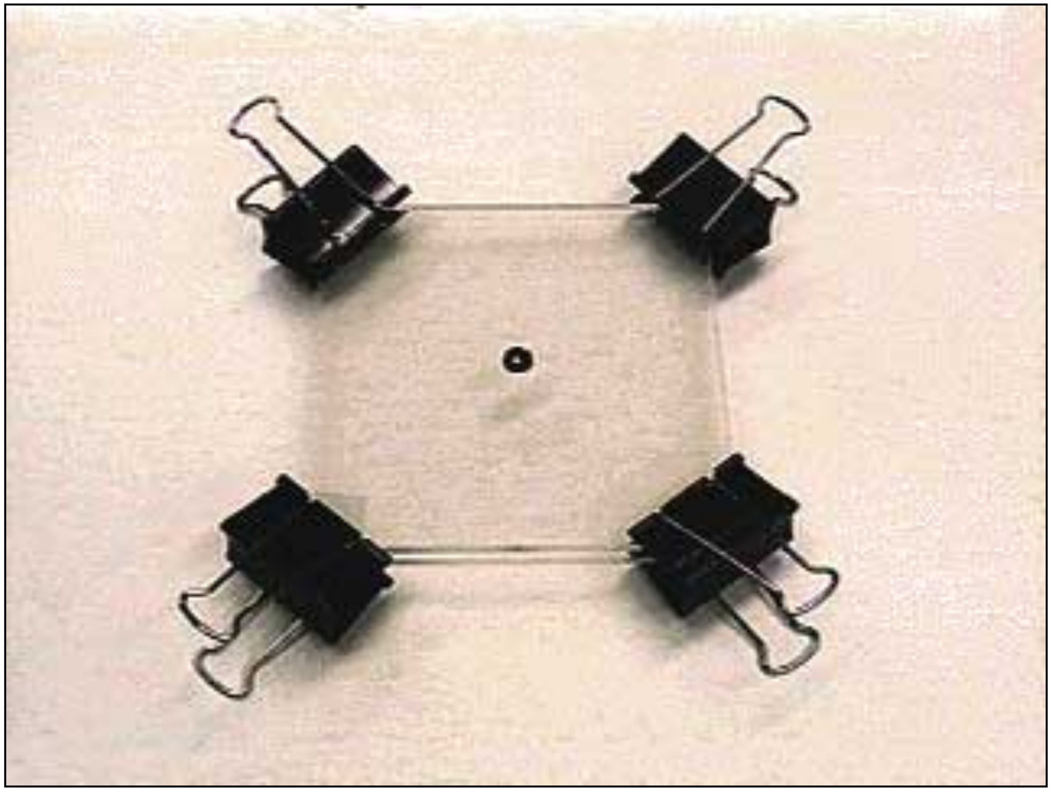
  $$DP= P_{interface} \text{ (air pressure is constant by comparison)}$$
  $$= T/R + P_0$$

  Where T is the surface tension parameter and R is the radius of curvature
- If we delve further into the equations, we find a number of insolvable equations. We therefore turn to numerical simulation. We use the monte carlo/random walkers method to do so.

Numerical Simulation/DLA

- Diffusion-Limited Aggregation, or DLA, is a simple computer simulation of the formation of clusters by particles diffusing through a medium that jostles the particles as they move. It essentially is the Monte-Carlo method to simulate the dendrite formation.
- Using this simulation, we can build up a large aggregate. **This process is called diffusion-limited aggregation because the growth of the cluster is governed by the particles' diffusion across the domain.**

Details of Numerical Simulation and the experiment



The Experiment:

- The Hele-Shaw Cell
- 2 different setups:
  - Air into Glycerol
  - Water into Glycerol
- Inject fluid at high pressure, many small fingers
- Inject fluid at low pressure larger fingers form

Problems…

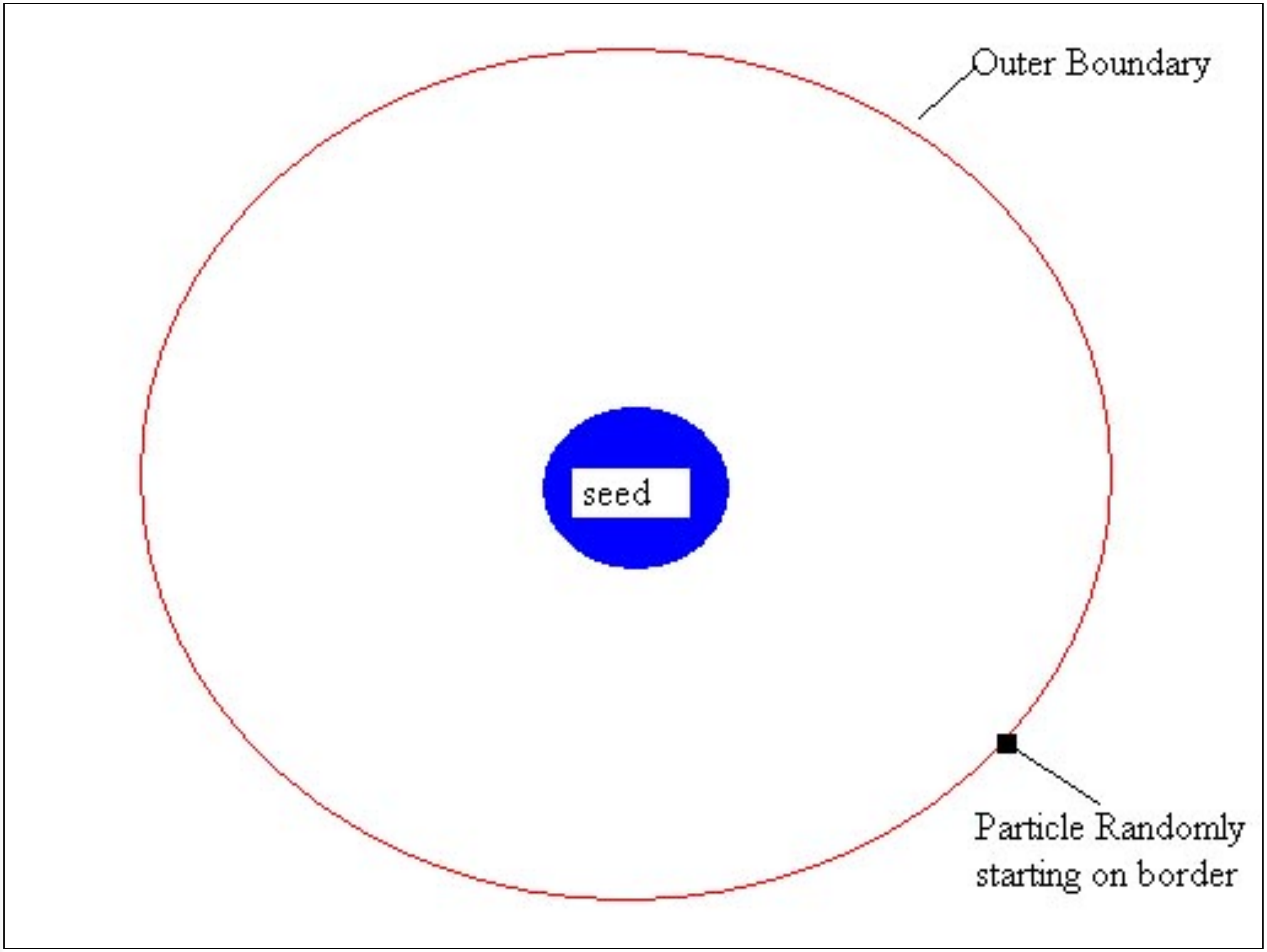
- Difficulty in getting tight seal, where fluid was injected
- Too little fluid, no ‘fingers’, too much fluid would break outer rim of glycerol
- Air bubbles in glycerol

Results…

- (play video of air into glycerol)
- (play video of water into glycerol)

The Numerics

- Had circular outer domain, lust like glycerol fluid in cell
- Started off with a seed – small circle in middle of domain
- Particles randomly generated on outer domain
- The particles then move randomly around
- Either hit seed or leave domain
- Need at least 10^5 to notice decent growth



Outer Boundary
seed
Particle Randomly
starting on border

The sticking rule

- 2 types
- 1st type is based on number of time particle hits figure
- The number of hits required to stick is predetermined before hand
- If particle doesn’t stick after hitting figure, it bounces off back into the domain until it hits and sticks or leaves the domain

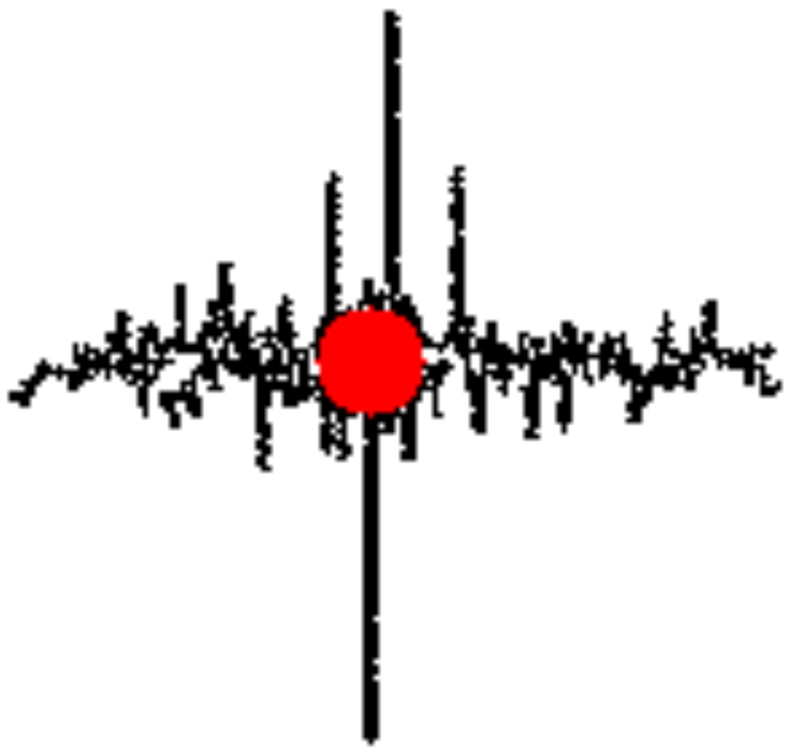
The sticking rule (2^{nd} type)

- Depends on the figure's curvature around the place where it hit
- To determine curvature simply count the of occupied spaces(N_l) in a circle of radius l centered on the particle
- $N_o = (l - 1) / 2l$
- $n_i = N_l / pl^2$
- $P(n_i) = A(n_i - n_o) + B$
- The smaller the value of A the more jagged the figure looks
- Larger values will make big bubbly figures

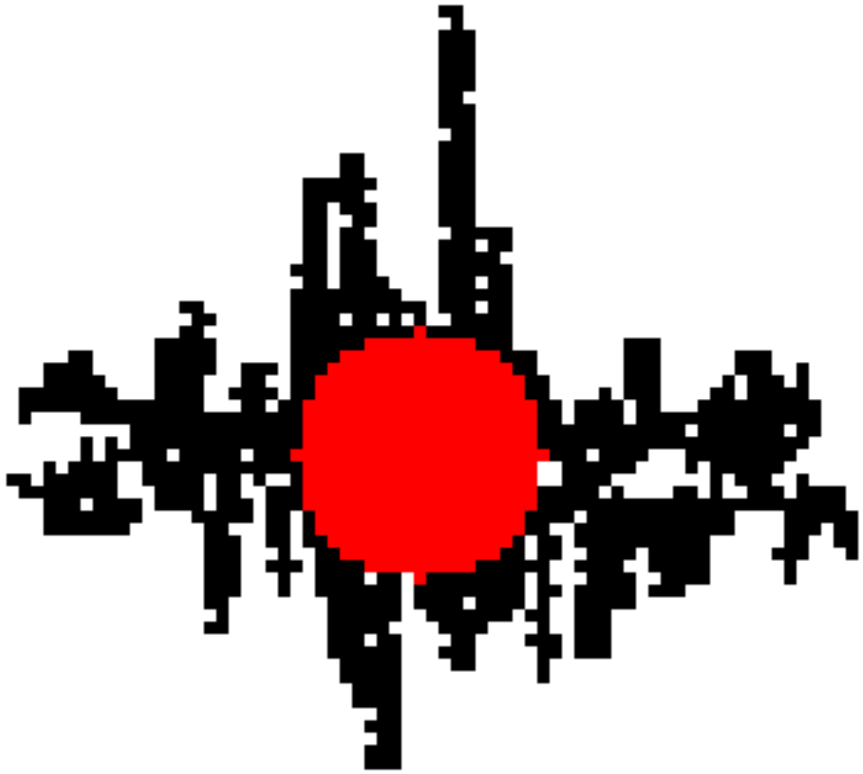
Surface Relaxation Method

- After a particle is chosen to stick to the figure where it sticks must be chosen carefully
- Using this method the particle is placed in a spot with the most neighboring spots occupied
- This will reduce ‘holes’ in the figure and overall better growth

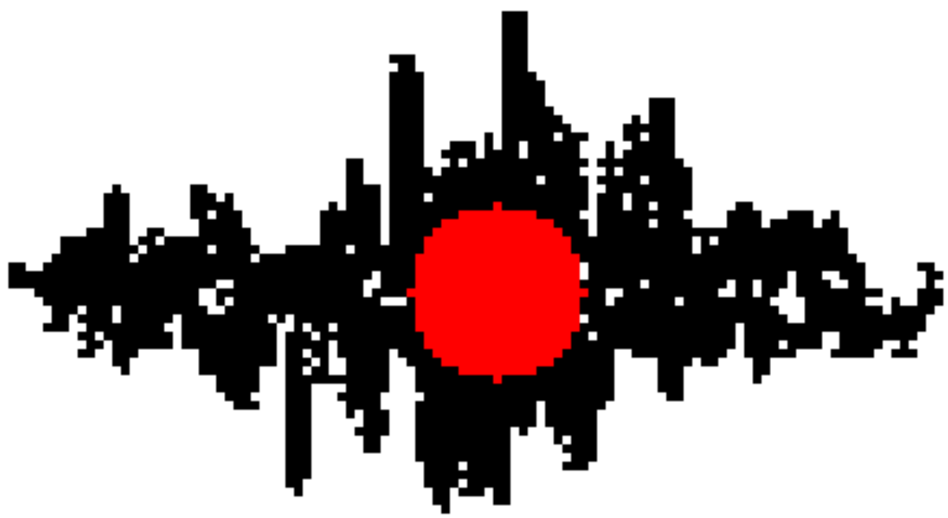
Particle Sticks on 1st Try



Particle Sticks on 3rd Try



Particle Sticks on 5th Try



Results…

- The output of the program is a text file with xy coordinates
- These coordinates are graphed pixel by pixel and displayed on the screen

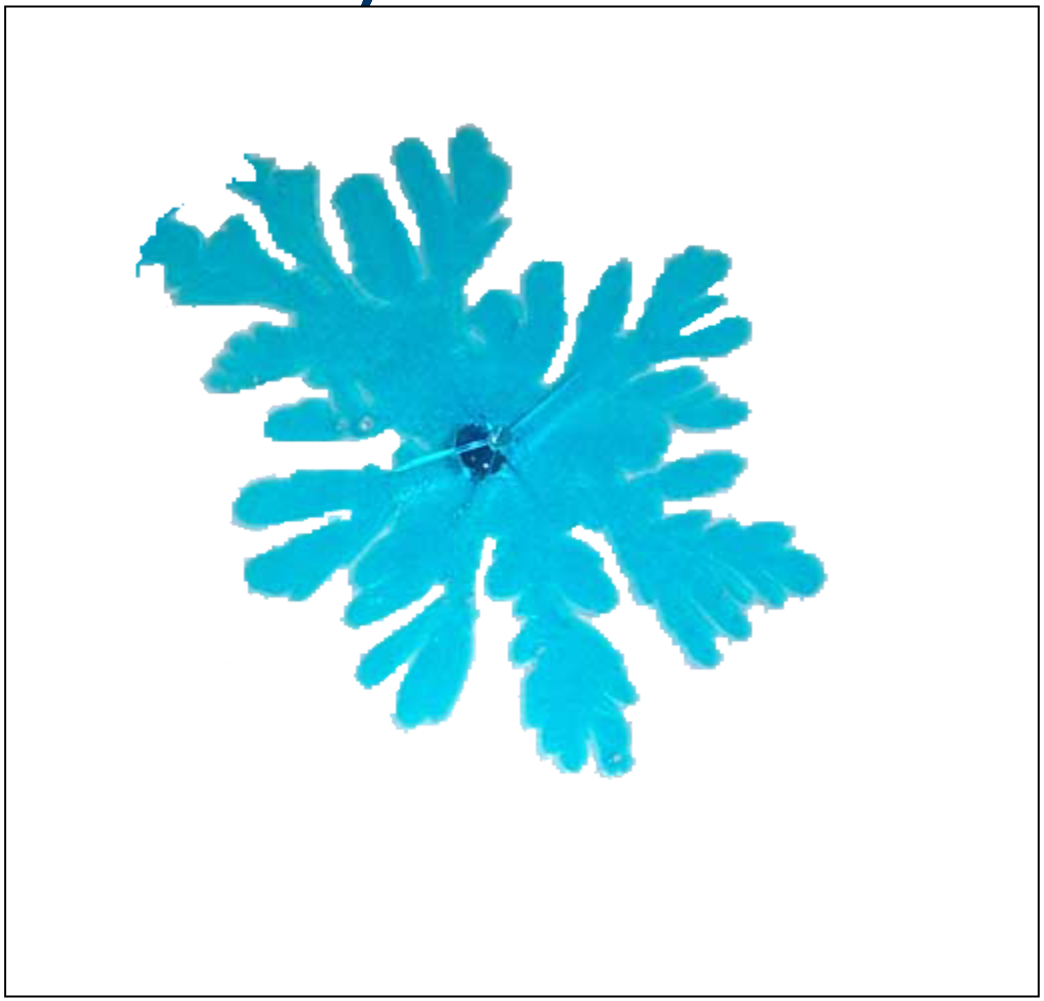
Indication of Fractal Nature

- Growth deep inside the fjords is very slow since a wandering particle must avoid contacting the walls in order to arrive deep inside: the branches screen the interior from additional growth.

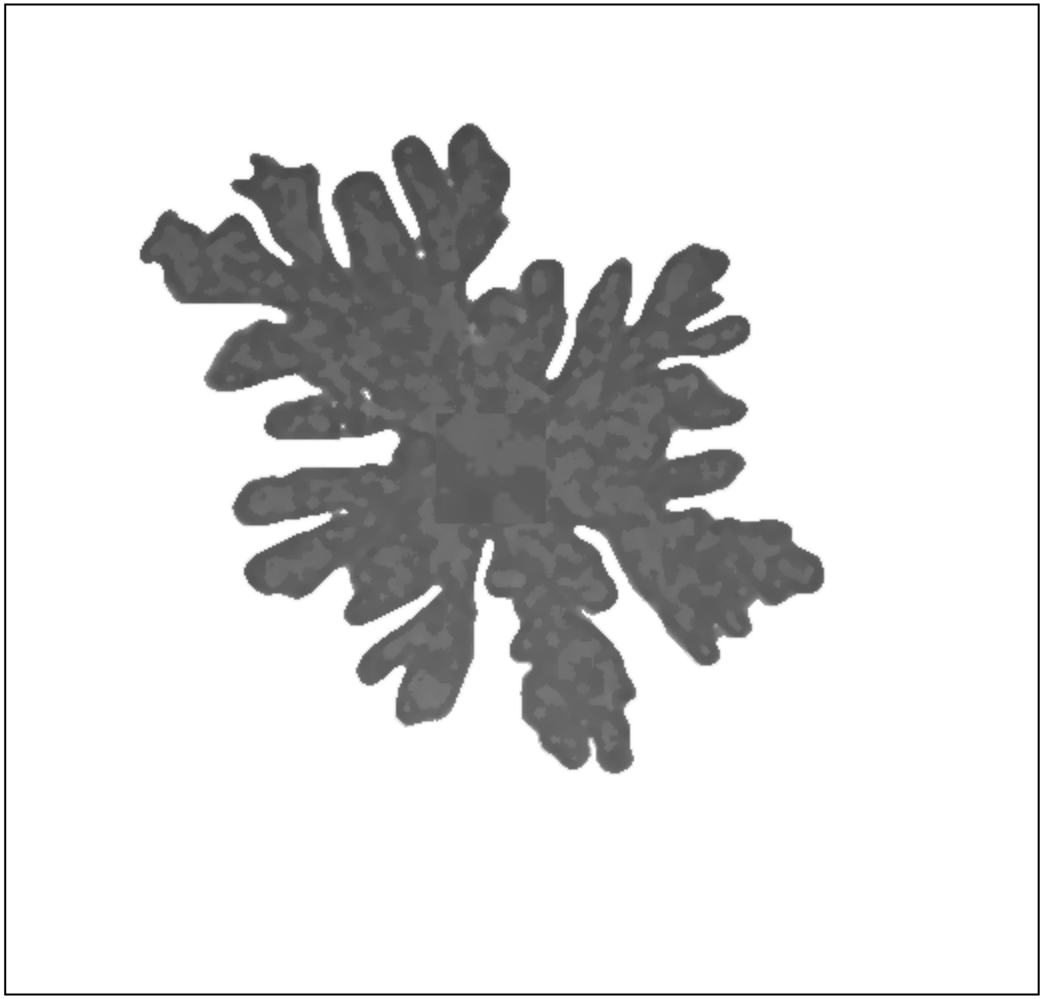
- This argument makes plausible that fjords persist once they form. To see how these fjords arise, consider their complement, the branches of the cluster. A single-cell bump on a straight edge of the cluster is not damped out by further growth, but rather is amplified because it has more growth sites (unoccupied neighbors) while each cell along the edge has only one growth site, and so the bump is more likely to capture a wandering particle. That is, initial fluctuations from the straight-line edge are likely to grow into larger branches, and the spaces between the branches are the beginnings of the fjords.

- This behavior is also exhibited along each branch: by the same process, bumps along a branch lead to the formation of smaller branches off the larger, suggesting that DLA clusters have fractal properties.

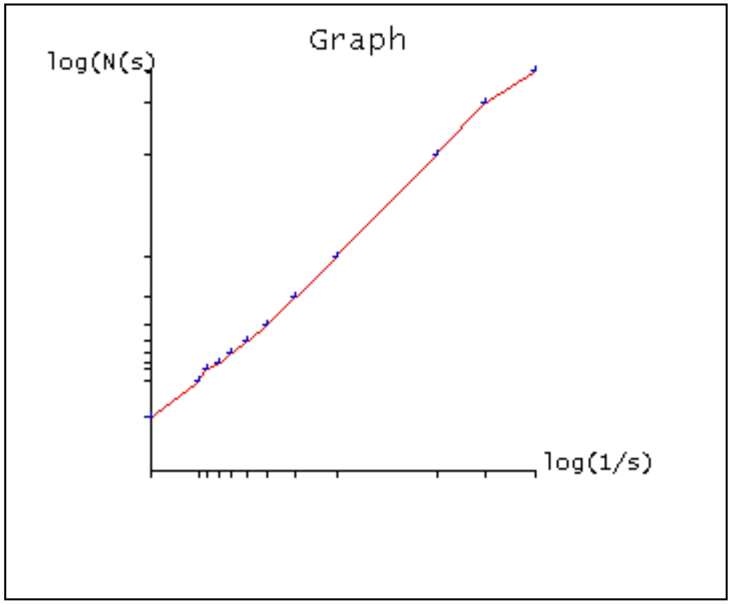
Analyzing clusters formed by DLA (using Fractal Dimension Calculator)



Grayscale Experiment Image

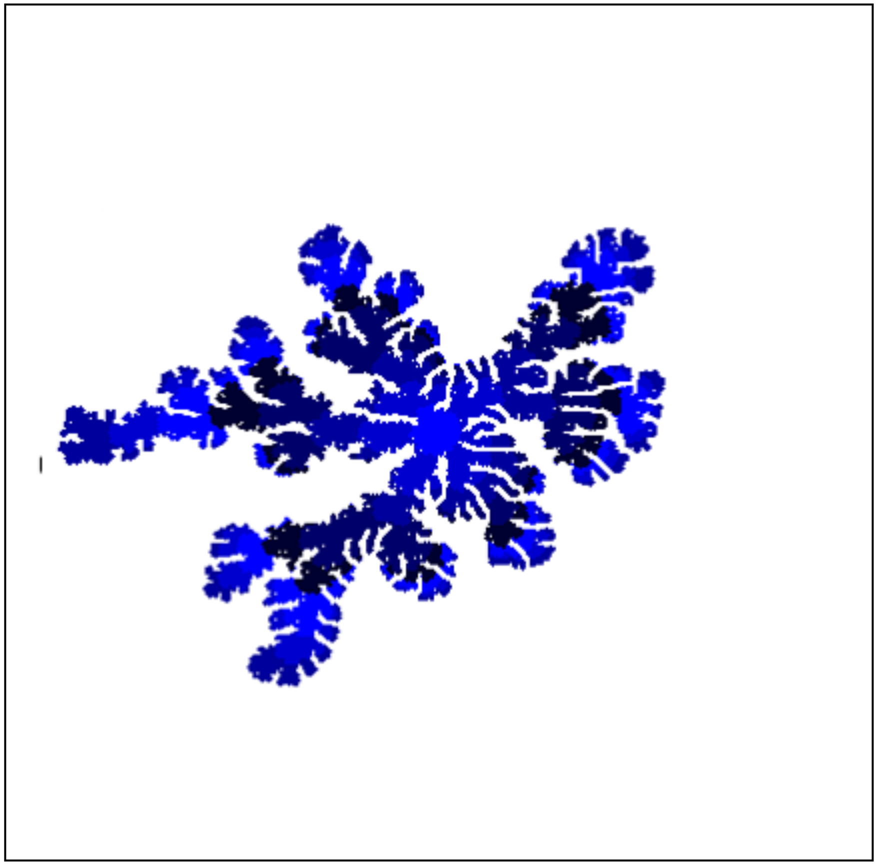


Box Dimension for experimental Image log N(e) Vs log (1/e)

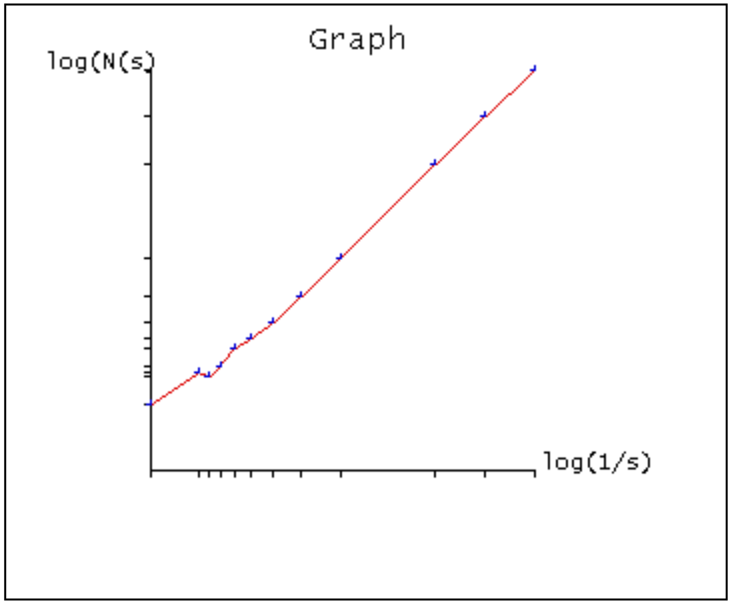


Box Dimension= 1.38629

Numerical Simulation Image



Box Dimension for Simulation Image log N(e) Vs log (1/e)



Box Dimension= 1.60944

Proof that DLA does simulate flow in a Hele Shaw cell

- Since Laplace Equation is satisfied by the probability distribution of random walkers, it is possible to draw an analogy between them. Also, DLA is described by the diffusion equation:

$$\frac{\partial C}{\partial t} = \upsilon \nabla^2 C$$

  where C is the concentration of particles as a function of position and time and n is the diffusion constant.

- With a steady flux of particle from a source that is far away from the aggregate of particles stuck, we obtain

$$\frac{\partial C}{\partial t} = 0$$

  resulting the diffusion equation to reduce to the Laplacian:
  Therefore, we can use it to simulate the aggregation in the fluid.

Conclusion

- DLA is an excellent tool to model the given problem and can be used for simulation of phenomena which exhibit such fractal growth patterns. E.g. Directional solidification, accumulation of particles on electrodes in electrolysis etc