DLA Simulations

Statement of Purpose

To simulate radial Hele Shaw flow of an air bubble expanding in a Newtonian fluid using Monte Carlo method (random walkers)/ Diffusion Limited Aggregation (DLA) and elucidate the fractal nature of the numerical method involved, so as to indicate the applicability of the process to other physical phenomena.

I. Introduction

The irreversible aggregation of small particles to form clusters is a central problem to many fields in applied science; examples are colloids and coagulated aerosols.¹ Often, the knowledge of behavior of such processes is critical to various industrial designs as it translates into expensive state of the art infrastructure. Therefore, it becomes absolutely necessary to study such phenomena and be able to predict them without having to indulge in

expensive lab simulations. Numerical Simulation has thus proven to be an effective method of choice. One such mechanism is Diffusion Limited Aggregation, more popularly known as DLA.

Diffusion-limited Aggregation (DLA) is an idealization of the process by which matter irreversibly combines to form dust, soot, dendrites and other random objects as in the case where the rate limiting step is diffusion of matter to the aggregate.²

II. Background Information

Dimensions³

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. For example, a rectangle is two-dimensional, while a cube is three-dimensional. Finite collections of objects (e.g., points in space) are considered 0-dimensional.

Objects that are "dragged" versions of zero-dimensional objects are then called onedimensional. Similarly objects, which are dragged one-dimensional objects, are twodimensional, and so on.

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.

Cover⁴

A family γ 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.

There are several branchings and extensions of the notion of topological dimension. <u>Implicit</u> 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.

<u>Hausdorff dimension</u>⁵: (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 and Fractal Dimensions⁶

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

Examples:



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.

 $M_D(S) = limit \quad \infty \quad ln N(\epsilon)$

$$\epsilon \rightarrow 0 r_k < \epsilon \ln 1/\epsilon$$

(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 .

But in practice box-dimensions are much easier to work with. For instance, the capacitydimension DC, defines a partition of the fractal into equally sized cubes with edge size ε

$$D_{\rm H} = \text{limit} \quad \frac{\ln N(\epsilon)}{\epsilon \rightarrow 0}$$
$$\epsilon \rightarrow 0 \quad \ln 1/\epsilon$$

 $N(\varepsilon)$ 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 the images obtained via numerical simulation and by actual experiments).

III. Experiment

The following figure shows a Hele-Shaw cell with its two plates of plastic separated by cover slips. In each corner there are two cover slips, one on top of the other..



Fluid is injected through the center hole. The space between the plates is fixed by the thickness of two cover slips, one on top of the other placed in each corner of the cell. In the experiment

- 1. We first injected glycerol through the central hole to fill the cell. After the cell was filled with glycerol, we injected colored water (blue).
- 2. We injected glycerol through the central hole to fill the cell. After the cell was filled with glycerol, we injected air

 $\frac{IV. \ Equations^7}{V = -b2 \ \nabla p / \ 12 \ \mu}$ where b= gap between the 2 pieces, and μ 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.

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:

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

where C is the concentration of particles as a function of position and time and v is the diffusion constant. With a steady flux of particle from a source that is far away from the aggregate of sticked particles 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.

$$\nabla^2 C = 0$$

V. Experimental Observations

As we inject one fluid into the glycerol (air or water) structures known as <u>fingers</u> form. These structures are also known as "dendrites", owing to their often highly branched structure. There are two key observations

- 1. When we inject fluid at high pressure, many small fingers form.
- 2. When we inject fluid at low pressure larger fingers form
- 3. Air in Glycerol does not dissolve, while water in glycerol does



Sample of Water (Blue) injected in Glycerol

VI. 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.

In order to simulate the experiment, we choose a circular outer domain, just like the glycerol fluid in Hele Shaw Cell.

♦ We start off with a seed – A small circle in the middle of domain

◆ Particles are randomly generated. The particles can then move randomly around

They either hit seed or leave domain

We need at least 10⁵ particles to notice decent growth. Weather or not a particle sticks to the seed, is determined by the sticking rule.



There are 2 types of sticking rules (used for purposes of this simulation) 1. <u>Based on number of times the particle hits figure</u>

The number of hits required to stick is predetermined. If a particle doesn't stick after hitting figure, it bounces off back into the domain. It can then hit the central seed again thus increasing the number of hits and sticks when the predetermined number is met, or it leaves the domain in which case it is invalidated.

2. <u>Based on the curvature of the central growing cluster around the location where it is hit</u> The second sticking rule is determined by curvature. We take a small circle of radius raround where the particle lands (r should be odd).

n1 = number of spaces occupies by particles from the figure / total number of available spaces in circle with radius *r*

NOTE: n1 < 1 (always) Now use n1 to determine the probability of sticking:

$$P(n1) = A (n1 - n0) + B$$

 $n0 = (r - 1) / 2r$

where B is a constant. A is an important factor for the equation. A represents the surface tension. The higher the value of A the higher is the surface tension the smoother the surface

(which means less surface area). For lower values of A you will get fractals which lead to higher surface area which means there is lower surface tension

Surface Relaxation Method

After a particle is chosen to stick, the place in the figure where it sticks must be chosen carefully. Surface Relaxation places the particle in a spot with the most neighboring spots occupied. This will reduce 'holes' in the figure and give an overall better growth We check the particles neighbors –1, 2 or 3 particles to the left and right and place the particle in the slot with the most adjacent neighbors. This would eliminate the holes. The more particles we check to the left and the right the longer it will take to complete a simulation. Checking two particles to the left and the right is sufficient to eliminate most of the holes— three particles and you get virtually no holes.

VII. Analysis

Continuing in this way described by numerical similuation, 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 grid.

Qualitative Analysis

Indication of the fractal Nature

• Obtaining such complicated patterns from simple rules may be surprising, but a qualitative understanding of some features is straightforward.

Growth deep inside the fjords (structures where between the dendrites) 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 three 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.

Reason for Mixing, Fingering (Fine and Broad):

- When we inject fluid at high pressure, many small fingers form while when we inject fluid at low-pressure larger fingers form. This is because of the higher surface tension in the former case, which causes high fingering.
- Air in Glycerol does not dissolve, while water in glycerol does. This is due to surface tension approaching zero in the latter case.

Quantitative Analysis (Using Fractal Dimension Calculator- FDC)

The fractal dimension calculator was used (designed Dr Paul Bourke at Swinburne University of Technology in Australia) to calculate the fractal dimension of the images obtained via the experiment and the simulation. This method makes use of the box dimension approach.



Grayscale Experiment Image

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





Box Dimension= 1.38629

Numerical Simulation Image

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



Box Dimension= 1.60944

VIII. Conclusion

In ideal experimental setups, where precision is taken care of to a much greater extent, the typical value of Fractal Dimension obtained for structures resulting from similar interfacial instability is of the order of 1.7. The results obtained numerically, closely parallel those (~1.6) while the experimental ones also come quite close (~ 1.4). Thus, we have established that DLA indeed does have fractal nature (supplemented by previous qualitative analysis). And it can be thus used for simulation of phenomena, which exhibit such fractal growth patterns. Eg Directional solidification, accumulation of particles on electrodes in electrolysis etc

References ^{1,2}T.A. Witten and L.M. Sander, Physical Review B, Volume 27, Page 5686 (1983) ^{3, 4, 5, 6} <u>http://www.mathworld.wolfram.com</u> ⁷ Shoudan Liang, Physical Review A, Volume 33, Page 2663 (1986) ⁸ <u>http://astronomy.swin.edu.au/~pbourke/fractals/fracdim/</u>