TSP Water Project Report

Snowflakes and Fractals

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Introduction

Snowflakes are among nature's most exquisite creations. Seemingly infinite in their intricacy, they hide beauty in amongst their complexities. It should come as no surprise then, that the mathematics behind snowflakes is arcane, but elegant and fulfilling.

This TSP project was concerned with exploring these wonders of nature and their properties, understanding the underlying physics and constructing representative models. The project was divided into two "teams"; the pure mathematics group considered the concepts behind fractals and their application to Lindenmayer systems, while the computing group considered computer modelling of snowflakes.

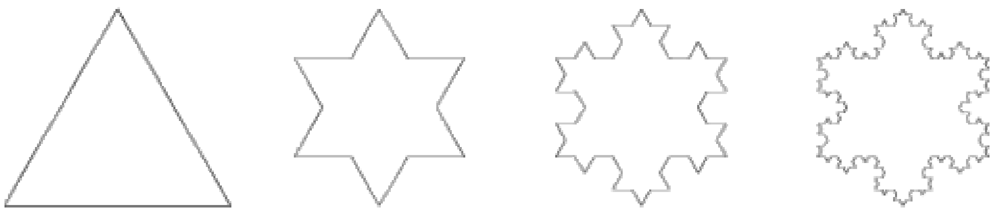
Mathematics Focus Group

The pure mathematics team considered Lindenmayer systems, an iterative method for fractal generation, linear algebra and metric spaces, required for analysis of the abstract properties of fractals.

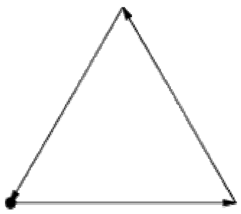
Lindenmayer Systems

Lindenmayer systems (or L-systems for brevity) were proposed by Aristid Lindenmayer in 1968 to provide models for the development of simple filamentous organisms such as plants. The simplest type of L-system is a D0L system, that is, a deterministic simple L-system.

For example, the Koch snowflake can be created via L-systems:



The snowflake is generated from an initial set of three lines forming an equilateral triangle:



The set of rules, which are used to replace each line, is as follows:

Mathematical Analysis of L-systems

DEFINITION L.1. An alphabet is a set of abstract symbols, usually finite and non-empty. The elements of an alphabet Σ are called letters or symbols, and a word over an alphabet Σ is a finite string consisting of zero or more letters of Σ. The set of all words over Σ is Σ^*.

DEFINITION L.2. A D0L system is a triplet $G = (\Sigma, h, \omega)$, where Σ is an alphabet, *h* is an endomorphism defined on Σ^* (that is, a bijective mapping $h:\ \Sigma \to \Sigma^*,\ a \to \alpha$), and ω (the axiom) is an element of Σ^*.

The graphical interpretation of L-systems is facilitated by the notion of a LOGO programming language-style turtle.

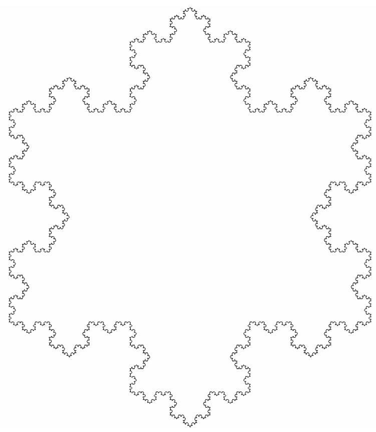
Given a step size *d* and an angle increment δ, the following commands are defined:

F — Move forward a step of length *d*. The turtle's state alters to (x', y', ϑ), where $x' = x + d\cos\vartheta$ and $y' = y + d\sin\vartheta$. A line segment between the points (*x*, *y*) and (*x*', *y*') is drawn.

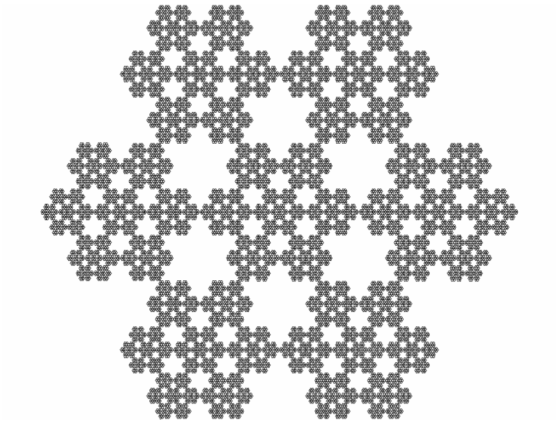
+ — Turn right by an angle δ. The turtle's state alters to $(x, y, \vartheta + \delta)$, assuming that the positive orientation of angles is clockwise.

− — Turn left by an angle δ. The turtle's state alters to $(x, y, \vartheta - \delta)$.

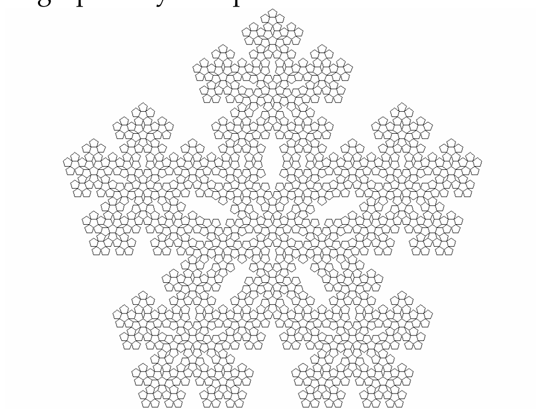
EXAMPLE L.1. The Koch Snowflake is defined by the D0L system $G = (\Sigma, h, \omega)$, where $\Sigma = \{F, +, -\}$, $h:\ F \to F + F - - F + F$, and $\omega = F - - F - -$. Here, $\delta = 60°$.



EXAMPLE L.2. A more accurate representation of a natural snowflake is given by the D0L system with angle $\delta = 60°$, $\Sigma = \{F, +, -\}$, $h:\ F \to F+F+F--F--F+F+F$, and $\omega = F+F+F+F+F+F--$.



EXAMPLE L.3. A snowflake shape is also represented by the D0L system $\Sigma = \{F, +, -, |\}$, $h:\ F \to F++F++F|F-F++F$, $\omega = F++F++F++F++F$, and angle $\delta = 36°$. The additional symbol | is graphically interpreted as a turn of $180°$.



Metric Spaces

Despite the intricacy and beauty of these fractals, the computer is limited to a finite number of iterations. So far, there has been no proof that these L-systems converge as the number of iterations approaches infinity nor any guarantee that the images the computer has produced are unique. To answer these objections, we employ metric spaces.

A metric space (X, d) is essentially a set X (of any mathematical objects – algebraic, geometric, or otherwise) over which "distance" is defined by a certain function d. Since we were dealing with essentially a sequence of images S_0, S_1, S_2, … where S_k is our snowflake after k iterations, we then looked at sequences within metric spaces. Specifically, we learned about Cauchy sequences, those for which the distance between x_n and x_m both in X is arbitrarily small for all large n, m. At this stage, we came across a theorem of considerable importance for the project:

Theorem: Every convergent sequence in a metric space is bounded, and has a unique limit.

The final definition that is required is that of a complete metric space: those in which every Cauchy sequence converges to an element in X.

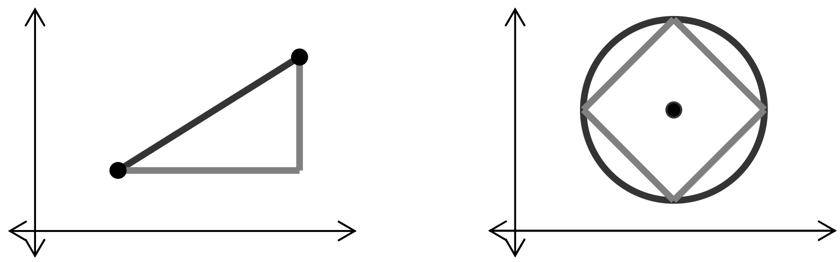
Sidebar 1: Metric Axioms

The distance function, $d(a,b)$ – the "distance" between a and b – must satisfy three axioms for all x, y and z in X:

1) Non-negativity: $d(x,y) \geq 0$, and $d(x,y) = 0$ iff $x = y$;
2) Axiom of Symmetry: $d(x,y) = d(y, x)$;
3) Triangle Inequality: $d(x,z) \leq d(x,y) + d(y,z)$.

Sidebar 2: Example Metrics

In $\mathbf{R}^2$, the *standard Euclidean metric* is given by the Pythagorean distance between two points (black). Alternatively, we could define $d(x,y) = |x_1 - y_1| + |x_2 - y_2|$, in which case a "circle" (the locus of all points equidistant from a fixed point) would be a diamond (grey).



Sidebar 3: Cauchy Sequences

A Cauchy sequence is formally defined as follows:

For every $\varepsilon > 0$ there exists an $N > 0$ such that $d(x_n, x_m) < \varepsilon$ for all n, $m > N$.

We then applied this theory to L-systems, using the complete Hausdorff metric space. The mathematics here was heavily entrenched with topological concepts, so we restricted and narrowed the Hausdorff metric to two-dimensional Euclidean space.

Applying the formula to determine the Hausdorff distance to the Koch snowflake, we found that the iterations were Cauchy sequences. Since the Hausdorff metric space is complete, this then proved that the Koch iterations converged to a compact 2D object, and that this limit was unique. In fact, this method could be adapted to all of the L-systems we considered, since any iteration could be illustrated geometrically, and hence a Hausdorff distance calculated.

In addition, metric spaces also allowed us to prove that the snowflake was bounded, and hence it has finite area. However, every iteration in the L-system increases the perimeter by a factor of $^4/_3$, and it must diverge to infinity. Fractals can have finite area, but infinite perimeter! Indeed, we see what the word "fractal" means – a "fractional dimension".

There is a method for calculating the dimension of a fractal created using L-systems. Given h (as described above), count the number of "F" characters, and this becomes d. Then, to determine s:

- Define constant δ as above.
- Define variables A (the angle) and D (the distance).
- Run through the symbols in the string h.
- If the symbol is
  - F; $D \to D + \cos[A]$
  - a +; $A \to A + \delta$
  - a -; $A \to A - \delta$
- When there are no more symbols, then $s = 1/D$

Dimension = $-\dfrac{\ln[d]}{\ln[s]}$

Computing Focus Group

The second group investigated fractal formation as a result of physical processes in contrast to the mathematicians, and used computation modelling of such physical processes to inspect their fractal properties.

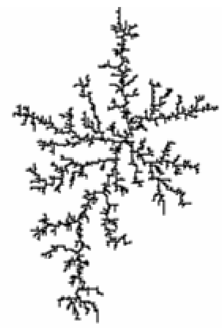
Basics of snowflake physics[1]

Snowflakes are not merely frozen water, for they exhibit crystalline structures, yet conversely are not entirely a single crystal. Rather, snowflakes are a cluster of snow crystals, each of which is formed by the condensation of water vapour on atmospheric dust particles.

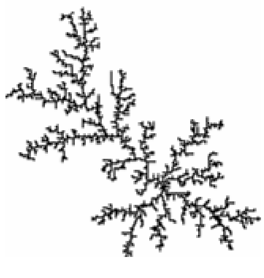
Questions are raised as to the conditions that allow for the formation of different types of snow crystals, and the formation of the macroscopic structure. Unfortunately, the physics underlying the connection between atmospheric variables and the resultant shape of snow crystals is still largely unknown. However, we do know some conditional relationships in a general sense. For instance, the formation of snow crystals depends on the surrounding temperature, the humidity (super-saturation), the necessary temperature conditions and the number of dust particles upon which to condense.

Once the condensation starts on a dust particle, due to the bending shape of the water molecule and its strong dipole, the formation of hydrogen bond gives the crystalline structure and enforces a bonding restriction. Then, as the clusters themselves collide into one another, the geometry of the water molecule restricts the bonding process. These very "simple" processes account for the myriad of snowflakes that have been observed.

First Hypothesis



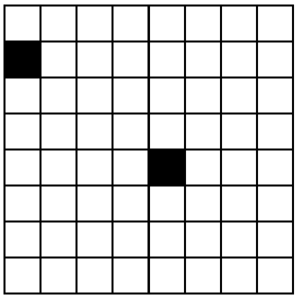
We postulated that the nature of the bonds between clusters formed the basis of the fractal geometry of the snowflake. That is, we conjectured that the restrictions on the bonding angle between clusters would manifest itself in the geometry of a fractal. In order to test this hypothesis, Diffusion Limited Aggregation (DLA), which produces random-looking "stochastic" fractals[2], was utilised.



DLA begins with a seed cluster. Free particles (clusters) are added to the system, and are made to undergo a random walk, until it collides with the cluster whereupon it bonds with the main cluster.

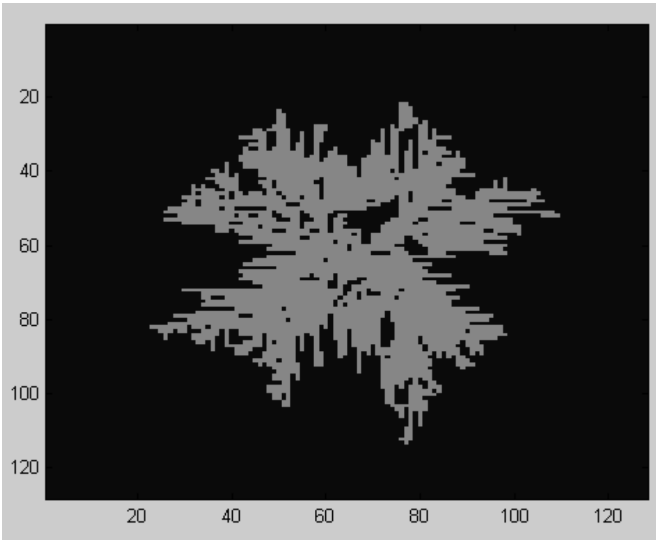
[1] "Snowflakes and snow crystals", http://www.its.caltech.edu/~atomic/snowcrystals/
[2] "What is a snowflake?" http://www.yptenc.org.uk/docs/factsheets/env_facts/snow.html

Grid-based DLA



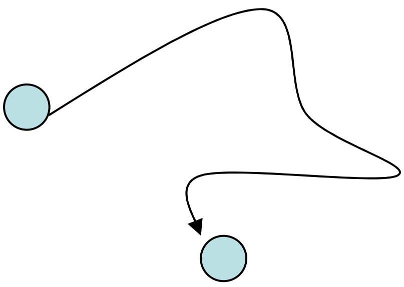
The first program, created in Matlab, allowed growth in four possible directions, namely upwards, downwards, to the left and to the right, chosen because rectilinear systems are convenient in computing. By using matrix values of '1' for existing particles and '0' for empty space, one could "grow" a fractal by switching values to simulate movement of particles. In this program, there were no restrictions on the bonding process to ensure 60-degree symmetry.

We then conjectured that a hexagonal or triangular grid would be of assistance, as this enforces the bond angle similar to the oxygen/hydrogen bond angle. In this case, there two new possible matrix values were introduced to represent semi-growth states, allowing us, effectively, to treat each grid location as two points, which together with weighted probabilities, allowed us to use conventional matrices to model growth on a triangular grid.



Despite the triangular grid system, the fractals produced do not resemble snowflakes.

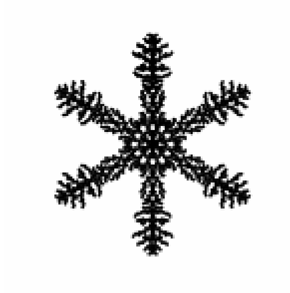
Second Hypothesis

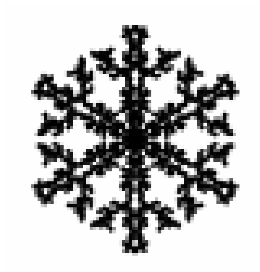


The result confirmed that the six-sided symmetry is not derived from simply a hexagonal lattice structure and random addition of clusters, rather, that the combination of clusters is deterministic. The clusters themselves are like three-dimensional jigsaws, such that each set of conditions forms similar clusters. As the flake falls through different conditions different clusters form, they combine in a "slotting" manner. In order to implement this preservation of symmetry, we began to investigate forced symmetry using a particle-based DLA model.

Particle-based DLA

Particle-based DLA utilises free particles that are not restricted to a particular lattice, this allows for the easy transposition of these particles to enforce symmetry. The implementation of particle-based DLA employed in this research project utilised an object-oriented programming language, providing high-level abstraction for the individual particles as they traverse a simulated environment.





To implement the jigsaw model, the location where the particle lands is noted, and eleven other particles are created in order to enforce plane and rotational symmetry. This encapsulates the idea that if the new cluster bonds to the main cluster, it is also likely to bond to the same sites with rotational symmetry assuming the cluster shapes are similar (due to the same environmental conditions). The images produced were perfectly symmetrical.

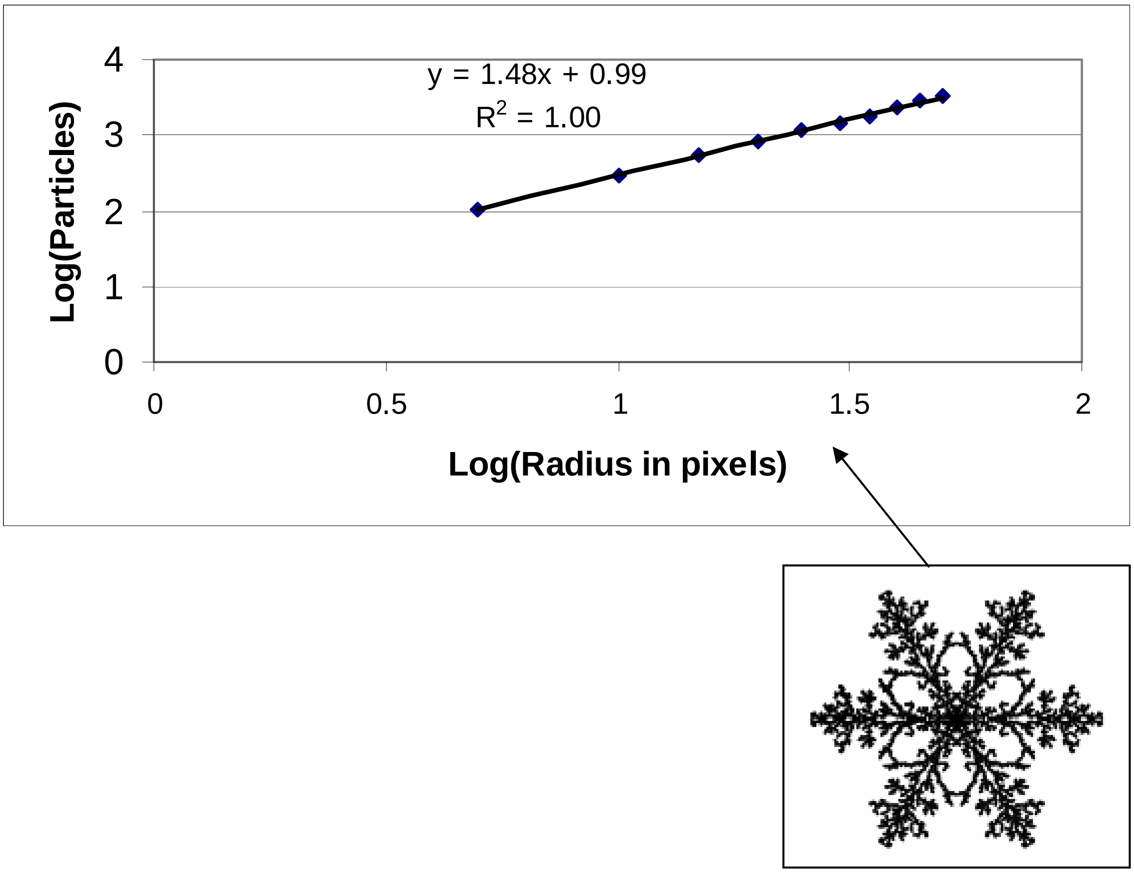
Several empirical analyses were performed on the snowflakes using this model. It was found that, although the area covered by the snowflake was roughly the same for each set of transforms, no relationship could be found between the numbers in the set of transforms for snowflakes with similar area. A small change in one variable produces unexpected results in another; this is a chaotic system.

Finally, the relationship $N(r) = k.r^d$ for the fractal's dimension[3] was investigated, where:

- $N(r)$ is the number of particles within a radius r of the centre
- d is the "mass" dimension (as we are dealing with particles)
- k is a fractal-specific constant

Rearranging the equation, we see that the mass dimension of the fractal is given by the gradient of the log-log graph. The fractals created by this program have been demonstrated to be truly DLA despite our modifications, as the R^2 value for the line of best fit is 1.00, indicating exact or almost exact fit to theory.

[3] "Fractal Geometry", http://classes.yale.edu/fractals/Panorama/Physics/DLA/DLA.html



On reflection, progression terms of three-dimensional modelling would have been ideal if there had been sufficient time, resources and skill, because that represents the true nature of snowflakes. Furthermore, the image resolution could have been increased to examine geometry on a microscopic level.

Conclusion

The TSP project "Snowflakes and Fractals" has led to an increased understanding of the way in which mathematics is able to model the environment around us. Mathematical principles were developed to place the physical ideas into context, and the computer simulation component evolved from disappointment to success. Fractals can be awe-inspiringly beautiful, and it is a wonderful opportunity for continuing popularisation of this area of science.