Analysis of the n-Dimensional Snowflake

Michael J. Lewis

Abstract. In this paper, the snowflake is modeled as a diffusion-limited aggregate. By means of the diffusion equation, we obtain the probability that, given unlimited time, a particle is absorbed by an aggregate in n-space, and subsequently, we verify this result through computer simulation for $n = 2, 3$. We then proceed to analyze the expected time required to capture for $n = 1, 3$ dimensions, thereby laying the groundwork for arbitrary n.

1. Introduction. The snowflake has been studied from a mathematical perspective for many years. It has been hypothesized that no two snowflakes are alike. This hypothesis is not unwarranted, as their crystalline structures exhibit the property of seemingly random branching patterns. This intrinsic property suggests a probabilistic model is appropriate.

Furthermore, a snowflake's geometry indicates self-similarity. That is, if we magnify a section of a snowflake, then the branching patterns that we observe in the crystalline substructure are similar to those we observe at the global level. Figure 1-1 illustrates this property; see [**3**] for more information on this image. Consequently, the process of forming a snowflake is aptly modelled by use of a stochastic fractal algorithm. The *diffusion-limited aggregate* (DLA) model, is one such model commonly applied to snowflakes, and this model is the focus of the present paper.

Figure 1-1. Notice the self-similarity in the snowflake's geometry.

Section 2 reviews the formulation of the DLA model and its physical justifications, then specifies the domain and formalizes the methodology that is utilized in Sections 3 – 5 for various capture analyses. Section 3 finds the probability of capture analytically for n-dimensions by use of the diffusion equation. Section 4 verifies the validity of the analytic solution. The final section, Section 5, determines the expected time until capture for both the 1-dimensional and 3-dimensional snowflake, and suggests the expected capture time for higher dimensions. This paper began as a term project for 18.354J. For a limited version of similar analysis, equivalently done through 18.354J though independently of this paper, [**1**] calculates the probability of capture in dimensions 2 and 3, but does not analyze the expected time to capture.

2. Modeling and Analyzing Snowflakes. This section focuses on reviewing what we know about the snowflake, and then proceeds to model its formation as a process known as diffusion-limited aggregation.

From a physical standpoint, a snowflake is little more than an aggregation of water molecules that have clumped together. Consider the following thought experiment: we have two particles in space with the same mass m, and m is relatively small, commonly on the order of nanograms. Let r be the distance between them, and G be the gravitational constant, which is approximately $6.67 \times 10^{-11}\ \mathrm{N \cdot m^2/kg^2}$. From Newton's gravity equation, we know that the gravitational forces between them is given by the formula

$$F_{\text{gravity}} = \frac{Gm^2}{r^2}.$$

Even at a distance on the order of micrometers, the particles' mutual gravitational attraction is on the order of 10^{-20} Newtons. From a potential perspective, the gravitational forces are so minute that they can be considered negligible; hence, the potential field is constant. Therefore, at least from the standpoint of energy, there is no one position that is favored over another; so from the particles' perspectives, all directions are equally preferable. This analysis is consistent with any number of particles. When a particle moves in a random walk at the infinitesimal length scale, we say it exhibits *Brownian motion*.

An obvious topic of interest is the coalescing of two clusters of particles into one. Conceptually, we expect there to be several considerations to take into account when we consider successful coalescing. Two noteworthy considerations are the following:

(1) the probability that two clusters collide,
(2) the probability that, having collided, the two amalgamate.

The first consideration is the central topic of discussion of the paper. The second refers to how ideal the contact site is, and this probability is a property of the local geometry of the site. Given the molecular structure of water, certain impact angles are preferred over others. This preference results in the symmetries we notice in natural snowflakes, and is known as the property of *facets*. Since snowflakes grow from a certain hexagonal primer, or geometric basis, the resulting structure necessarily exhibits similarity on the larger scale. This property is readily apparent in Figure 2-1. As above, see [**3**] for more information on this snowflake image.

Figure 2-1. The hexagonal primer in this snowflake is very apparent.

The property of facets not withstanding, since the particles move in Brownian motion, their probability density functions can be modelled via the *diffusion equation* [**4**, pp. 14–15]

$$\frac{\partial U}{\partial t} = \mathcal{K} \nabla^2 U \tag{2-1}$$

where $\mathcal{K}$, known as the *diffusion coefficient*, is a constant that is indicative of the characteristic length and characteristic velocity of the system being modelled. The name of this model, the *diffusion-limited aggregate*, stems from the fact that the aggregation of the particles is limited by the process of diffusion.

We wish to devise a method for analyzing the DLA, so that we can both find the probability a particle is captured by the aggregate and verify our analysis through computer simulation. A common way of analyzing the snowflake is to proceed from the perspective of the central aggregate. By assumption, all the particles are moving in Brownian motion: if we choose the origin to be the center of the aggregate, then the remaining particles still exhibit Brownian motion, and therefore the diffusion equation remains applicable.

Therefore, consider the following simplified system. Let the radius r be the Euclidean norm of n-dimensional position vector $\mathbf{x} = (x_1, \ldots, x_n)$ in the standard Euclidean space with the origin where the central aggregate is placed. Let R_0 be the radius at which particles are released to diffuse through the air. Let the aggregate's surface be an n-sphere, for simplicity, with radius R_a less than R_0. Since we wish to verify our model on the computer, we wish to consider a finite domain in which the particles diffuse. Let R_k be the radius at which the particle is assumed to have wandered from the local region and cannot attach to the aggregate; of course, R_k is greater than R_0. For simplicity, we henceforth refer to the outer shell with radius R_k as the *kill surface*, and R_k as the *kill radius*. This domain is depicted in Figure 2-2 shown below. By formulating the system in this manner, computation time can be saved while maintaining realistic properties. Physically, we wish to consider the entirety of $\mathbb{R}^n$, and so we can chose to take the limit as $R_k \to \infty$.

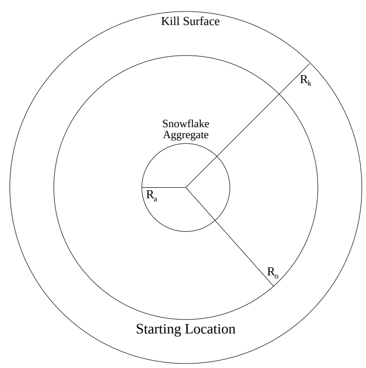

Figure 2-2. Domain for analyzing the DLA.

3. Analyzing Probability of Capture. As stated in Section 2, the evolution of the probability density function as a function of time for the particles can be described by the diffusion equation (2-1). This section considers the probability that, given ample time, a particle will collide with an aggregate in n-dimensions.

Consider the following situation: there is a constant source of particles at radius R_0, which maintains a constant concentration of particles Ω. We assume the aggregate and the kill surface are perfect absorbers, and therefore the concentrations at these surfaces must necessarily vanish. Assuming that we have a large number of particles, we expect their concentrations to converge to their probability density functions, and therefore their concentrations at a particular point $\mathbf{x}$ at time t can be quantified by a function $U(\mathbf{x}, t)$.

Recall that the Laplacian is defined the following way in Euclidean space:

$$\nabla^2 = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}. \tag{3-1}$$

A function $f(\mathbf{x})$ is said to be *harmonic* in a domain D if it satisfies the *Laplace Equation* [**4**, p. 16]:

$$\nabla^2 f(\mathbf{x}) = 0 \text{ in D}. \tag{3-2}$$

By symmetry, we expect the concentrations of the particles to be equivalent at any given radius. Consequently, we expect $U = U(r, t)$. By means of the chain rule and properties of the Euclidean norm, we obtain the following equations:

$$\begin{aligned} \frac{\partial U}{\partial x_i} &= \frac{\partial U}{\partial r} \cdot \frac{\partial r}{\partial x_i} \quad \text{and} \\ \frac{\partial r}{\partial x_i} &= \frac{x_i}{r} \quad \text{for } 1 \leq i \leq n. \end{aligned}$$

Using these equations, we discover the Laplacian of U is given by the following formula:

$$\nabla^2 U = \frac{\partial^2 U}{\partial r^2} + \frac{n-1}{r} \cdot \frac{\partial U}{\partial r}. \tag{3-3}$$

Since the source of particles at R_0 maintains a constant influx of particles, we expect the system to reach a steady state. By *steady state*, we mean that concentrations at all points are constant in time, or in mathematical terms

$$\frac{\partial U}{\partial t} = 0. \tag{3-4}$$

By combining (2-1) and (3-4), we find the concentration U of the particles are harmonic in the domains $D1 : R_a \leq r \leq R_0$ and $D2 : R_0 \leq r \leq R_k$ with $U = 0$ at $r = R_a$, R_k and $U = \Omega$ at $r = R_0$.

We can now rewrite the Laplace Equation for U using Equation (3-3), resulting in the following formula:

$$\frac{d^2 U}{dr^2} + \frac{n-1}{r} \cdot \frac{dU}{dr} = 0 \text{ in } D_1 \text{ and } D_2\ . \tag{3-5}$$

Notice that the partial derivatives have converted to standard derivatives, as a result of (3-4).

Using the governing partial differential equation in (3-5), with the defined boundary conditions in our system, we obtain the following concentration distributions: if $n = 2$, then

$$U(r) = \begin{cases} \Omega \ln(r/R_a) \big/ \ln(R_0/R_a) & \text{for } R_a \leq r \leq R_0, \\ \Omega \ln(R_k/r) \big/ \ln(R_k/R_0) & \text{for } R_0 \leq r \leq R_k; \end{cases}$$

otherwise,

$$U(r) = \begin{cases} \Omega \dfrac{R_a^{2-n} - r^{2-n}}{R_a^{2-n} - R_0^{2-n}} & \text{for } R_a \leq r \leq R_0, \\ \Omega \dfrac{R_k^{2-n} - r^{2-n}}{R_k^{2-n} - R_0^{2-n}} & \text{for } R_0 \leq r \leq R_k. \end{cases}$$

Since Ω is positive, the concentration function U is nonnegative everywhere, as a density function should be.

The rate at which the particles are being captured can be understood to be the total flux at the boundaries. Conceptually, the flux is the rate of flow of fluid through a surface S. Mathematically, the flux through a surface S is defined in the following manner:

$$flux_S \equiv \oint_S \mathcal{K}\nabla U \cdot \mathbf{n} dS \tag{3-6}$$

where $\mathbf{n}$ is the unit normal vector pointing out of the surface element dS and ∇U is the gradient of U.

In the system we are considering, we find the following values along our boundaries:

$$\mathcal{K}\nabla U \cdot \mathbf{n} = -\mathcal{K} \cdot \left.\frac{dU}{dr}\right|_{r=R_a} \tag{3-7}$$

along the aggregate's surface, and likewise

$$\mathcal{K}\nabla U \cdot \mathbf{n} = \quad \mathcal{K} \cdot \left.\frac{dU}{dr}\right|_{r=R_k} \tag{3-8}$$

along the kill surface. These values are constant along their respective surfaces. Taking a step back, we find that the surface area of an n-sphere of radius r is $S_n r^{n-1}$ where

$$S_n = \begin{cases} \dfrac{2^{\frac{n+1}{2}}\pi^{\frac{n-1}{2}}}{(n-2)!!} & \text{for } n \text{ odd,} \\ \dfrac{2\pi^{n/2}}{(\frac{1}{2}n-1)!} & \text{for } n \text{ even.} \end{cases}$$

Here, the notation $n!!$ denotes the *double factorial* of n, where

$$n!! = \begin{cases} n \cdot (n-2) \ldots \cdot 3 \cdot 1, & \text{for } n \text{ odd;} \\ n \cdot (n-2) \ldots \cdot 4 \cdot 2 & \text{for } n \text{ even.} \end{cases}$$

See [**2**] for more details on the derivation.

As is seen in the final capture analysis, however, the value of the constant is insignificant. The proportionality of the surface area to r^{n-1} is the key factor.

Conceptually, we expect the probability of capture to be the flux through the aggregate's surface compared to the total flux out of the system:

$$P_{\text{capture}} = \frac{\text{flux}_{R_a}}{\text{flux}_{R_a} + \text{flux}_{R_k}}. \tag{3-9}$$

Here, we choose flux_{R_a} to be the total flux through the aggregate's surface, and flux_{R_k} to be the total flux through the kill sphere's surface. By using our above equalities (3-6), (3-7), and (3-8), we can see that

$$\begin{aligned} \text{flux}_{R_a} &= -S_n R_a^{n-1}\mathcal{K}\left.\frac{dU}{dr}\right|_{r=R_a}, \\ \text{flux}_{R_k} &= \quad S_n R_k^{n-1}\mathcal{K}\left.\frac{dU}{dr}\right|_{r=R_k}. \end{aligned} \tag{3-10}$$

Having obtained both equations for the overall flux, and the analytic solutions for the steady-state case, we can now calculate the individual fluxes. For the aggregate's surface, the total flux is given by

$$\text{flux}_{R_a} = \begin{cases} -\dfrac{S_n \mathcal{K}\Omega}{\ln(R_0/R_a)} & \text{for } n = 2, \\ \dfrac{S_n \mathcal{K}\Omega(2-n)}{R_a^{2-n} - R_0^{2-n}} & \text{otherwise;} \end{cases} \tag{3-11}$$

and the total flux for the kill surface is

$$\text{flux}_{R_k} = \begin{cases} -\dfrac{S_n \mathcal{K}\Omega}{\ln(R_k/R_0)} & \text{for } n = 2, \\ \dfrac{S_n \mathcal{K}\Omega(2-n)}{R_0^{2-n} - R_k^{2-n}} & \text{otherwise.} \end{cases} \tag{3-12}$$

As a result of (3-9), (3-11), and (3-12), the probability of capture is the following:

$$P_{\text{capture}} = \frac{1}{1 + R^*}$$

where

$$R^* = \begin{cases} \dfrac{\ln(R_0/R_a)}{\ln(R_k/R_0)}, & \text{for } n = 2; \\ \dfrac{R_a^{2-n} - R_0^{2-n}}{R_0^{2-n} - R_k^{2-n}}, & \text{otherwise.} \end{cases}$$

As is apparent, the S_n factored out, and therefore its value is inconsequential in deriving this solution.

By taking the limit $R_k \to \infty$, we obtain

$$P_{\text{capture}}^{\infty} = \begin{cases} 1 & \text{for } n = 1 \text{ or } 2, \\ \left[\dfrac{R_a}{R_0}\right]^{n-2} & \text{for } n \geq 3. \end{cases}$$

where the '∞' indicates that we have performed the limit.

The obvious result of interest here is that the particles collide with the snowflake with certainty in the case $n = 1, 2$, yet a particle's chances of collision with the snowflake decrease geometrically as its degrees of freedom increase for larger n.

4. Numerical Verification. In order to verify the above analysis, various Matlab simulations with particles performing random walks in two and three dimensions were performed for the system described in Section 2. The expected probabilities of capture are graphed alongside the observed in Figures 4-1 and 4-2. As can be seen, the results appear to follow very closely with the analytic solution for P_{capture} from Section 3.

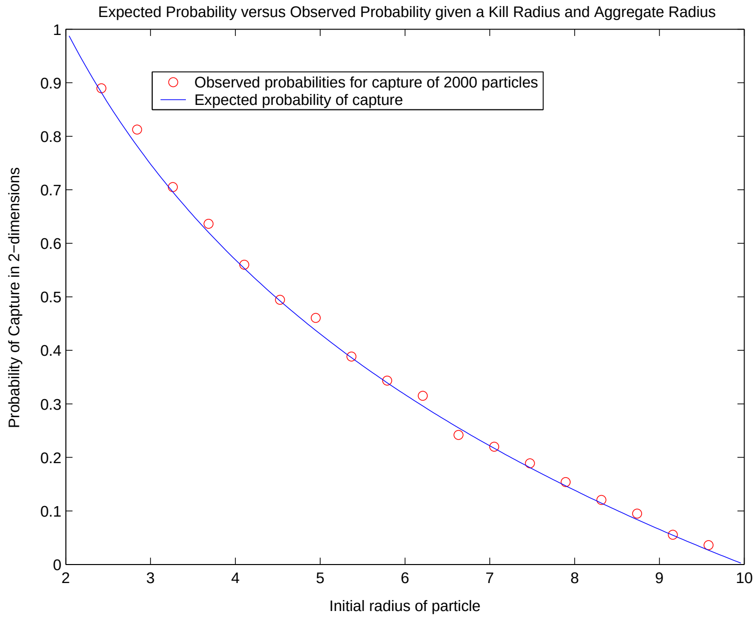

Figure 4-1. Numerical capture probabilities in 2-dimensions.

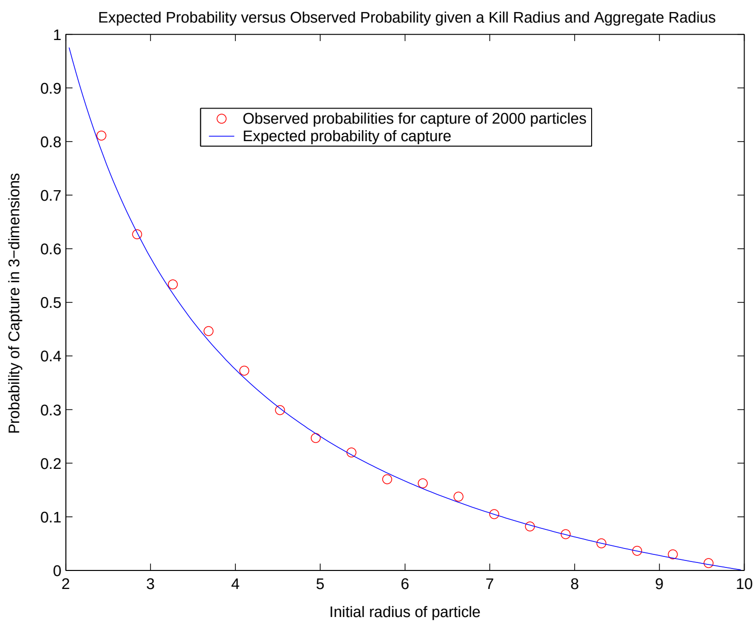

Figure 4-2. Numerical capture probabilities in 3-dimensions.

5. Expected Time to Capture Analysis. In Section 3, we solved for the probability a particle is captured given sufficient time. We now revisit the analysis with more interest in how much time is required. Thus we find the expected amount of time that is required for a particle to be captured in 1 dimension and in 3 dimensions.

In this situation, we consider the case where initially all the particles are placed at radius R_0. Thus, we have the initial condition

$$U(r,0) = M_n \cdot \delta(r - R_0) \tag{5-1}$$

where $\delta(x)$ denotes the dirac measure, M_n is a normalizing coefficient in n-dimensions (M_1 obviously being 1), and U satisfies

$$\frac{\partial U}{\partial t} = \mathcal{K} \cdot \left(\frac{\partial^2 U}{\partial r^2} + \frac{n-1}{r} \frac{\partial U}{\partial r} \right), \tag{5-2}$$

which results from (2-1) and (3-3).

For some dimension n, diffusion coefficient $\mathcal{K}$, and domain $\{ R_a \leq r \leq R_k \}$, let U_1 and U_2 be functions that each satisfy the given PDE (5-2) and initial condition (5-1) and vanish on the boundary. Notice that the function $U = U_1 - U_2$ also satisfies (5-2) and the zero boundary conditions, yet vanishes at t = 0. Since U is identically zero for $t = 0$, all space derivatives of U must necessarily be 0 initially, and subsequently $\frac{\partial U}{\partial t}$ is identically zero for $t = 0$ as a result of satisfying the PDE. Therefore, U is identically 0, and $U_1 = U_2$, and thus we establish the uniqueness of the solution to the system for each n.

For simplicity of calculation, let the first dimension we consider be $n = 1$. Then the PDE becomes the 1-dimensional diffusion equation. The well-known Green's function for the diffusion equation is

$$G(r,t) = \frac{1}{\sqrt{4\pi\mathcal{K}t}} \exp\left[\frac{-(r-R_0)^2}{4\mathcal{K}t} \right].$$

This solution satisfies the initial condition (5-1), yet holds to the domain of the entire real line. However, by using the method of images, which involves the principle of superposition, we can find the solution in our system to be a linear combination of two separate Green's functions:

$$U(r,t) = \frac{1}{\sqrt{4\pi\mathcal{K}t}} \left[\exp\left[\frac{-(r-R_0)^2}{4\mathcal{K}t} \right] - \exp\left[\frac{-(r+R_0-2R_a)^2}{4\mathcal{K}t} \right] \right] \tag{5-3}$$

The subsequent rate of flux at $r = R_a$ is therefore equal to

$$f(t) = \frac{R_0 - R_a}{t\sqrt{4\pi\mathcal{K}t}} \exp\left[\frac{-(R_0-R_a)^2}{4\mathcal{K}t} \right]. \tag{5-4}$$

This rate of flux is equal to the rate at which the particles are captured by the aggregate. As such, we find that the total percentage of particles caught is

$$\int_0^\infty f(t)dt = 1.$$

Thus all particles are inevitably caught. This conclusion agrees with our capture analysis for $n = 1$.

Since we trying to find the expected time of capture, we wish to find the expected value for $f(t)$, or

$$E\left[f(t)\right] = \int_0^\infty t \cdot f(t)dt = \int_0^\infty \frac{R_0 - R_a}{\sqrt{4\pi\mathcal{K}t}} \exp\left[\frac{-(R_0-R_a)^2}{4\mathcal{K}t} \right] dt.$$

However, for large t, it is apparent that the integrand $t \cdot f(t)$ decreases at a rate proportional to $t^{-\frac{1}{2}}$, or in symbols $t \cdot f(t) \propto t^{-\frac{1}{2}}$, and therefore the integral does not converge. Hence, the expected capture time for a particle exhibiting Brownian motion in one dimension is infinite.

Having solved the radially symmetric diffusion equation for our domain in the one-dimensional case, let us cosider a new function V(r,t) such that

$$U(r,t) = \frac{r}{M_3} \cdot V(r,t),$$

where $U(r,t)$ comes from (5-3), and M_3 stems from (5-1) for $n = 3$. Given that we know $U(r,t)$ satisfies (5-2) for $n = 1$, namely

$$\frac{\partial U}{\partial t} = \mathcal{K} \cdot \frac{\partial^2 U}{\partial r^2},$$

we find that this new function $V(r,t)$ satisfies the PDE

$$\frac{\partial V}{\partial t} = \mathcal{K} \cdot \left(\frac{\partial^2 V}{\partial r^2} + \frac{2}{r} \frac{\partial V}{\partial r} \right).$$

This is readily recognised to be Equation (5-2) for $n = 3$. Furthermore, given that $U(r,t)$ disappears at $r = R_a$ for all t, we know $V(r,t)$ also satisfies this boundary condition. Likewise, $V(r,t)$ resembles a dirac spike at $t = 0$. Thus the only concern left is the normalizing factor M_3. By integrating in spherical coordinates, we can find that we can normalize $V(r,t)$ at $t = 0$ by setting

$$M_3 = \frac{1}{4\pi R_0}.$$

Thus, we find the solution for the 3-dimensional radially symmetric diffusion equation for our domain and boundary conditions to be

$$V(r,t) = \frac{1}{4\pi R_0 r \sqrt{4\pi \mathcal{K} t}} \left[\exp\left[\frac{-(r-R_0)^2}{4\mathcal{K}t} \right] - \exp\left[\frac{-(r+R_0-2R_a)^2}{4\mathcal{K}t} \right] \right] \tag{5-5}$$

By making use of (3-10), and noting $S_3 = 4\pi$, we find that the flux at the aggregates surface in the 3-dimensional case to be

$$g(t) = \frac{R_a}{R_0} \frac{R_0 - R_a}{t\sqrt{4\pi \mathcal{K} t}} \exp\left[\frac{-(R_0 - R_a)^2}{4\mathcal{K}t} \right]. \tag{5-6}$$

It is readily observable that $g(t) = \frac{R_a}{R_0} \cdot f(t)$ for $f(t)$ defined in (5-4). Furthermore, we see that the total flux through the aggregate surface over all time is

$$\int_0^\infty g(t)dt = \int_0^\infty \frac{R_a}{R_0} f(t)dt = \frac{R_a}{R_0},$$

which coincides with capture analysis for $n = 3$. Since $g(t)$ is only a scaling factor different from $f(t)$, we again observe that the expected time to capture is infinite.

Conceptually, we should expect that this behavior is no different in any dimension n for the following reasoning: it is apparent from the probability of capture analysis that as the the number of dimensions increases, and consequently the number of degrees of freedom for the particles to move in increases, capturing appears to take even longer, relatively speaking, in the larger dimensions, and is consequently less likely. Therefore, we should expect the characteristic time scale for a snowflake formation to be very large in any dimension.

This analysis explains why snowflakes only form in the extreme conditions inside a cloud. In a cloud, the temperatures are considerably lower than those at the Earth's surface, and the number of particles amassed in the local region is considerably larger. Given this favorable environment, the particle capture rate, or more specifically the rate of formation of the snowflake, should be considerably higher than it would be elsewhere. These conditions are apparently sufficient to offset the otherwise large capture times per particle.

Acknowledgements

The author wishes to thank his advisor, Professor Steven Kleiman, for his patience and advice in writing and editing this article. He also wishes to thank Professor Thomas Peacock, his mentor in 18.354J, Nonlinear Dynamics II: Continuum Systems, for suggesting this problem as a class project. His support in constructing the problem mathematically was pivotal.

References

[**1**] Aristoff, Jeffrey M., *The Diffusion-Limited Aggregate*, MIT Undergraduate Journal of Mathematics **6** (2004), 1–9.

[**2**] "Wolfram MathWorld, the web's most extensive mathematics resource. Hypersphere entry," `http://mathworld.wolfram.com`, accessed 5/2004.

[**3**] "SnowCrystals.com. Snow Crystal Photo Gallery I," `http://www.its.caltech.edu/~atomic/snowcrystals`, accessed 12/2008.

[**4**] Strauss, Walter A., "Partial Differential Equations: An Introduction," John Wiley & Sons, Inc., 1992.