Computational Analysis of Diffusion as a Stochastic System

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Abstract

Computer simulations are used to model diffusion as a stochastic process. Random walks in one and two dimensions are compared to normal distributions. Diffusion-limited aggregation is modeled in two and three dimensions, and mass dimension is compared to literature values.

Introduction

Randomness serves as a core to biophysics. When dealing with particles on the scale of molecules, predicting the states of large systems can be precisely accomplished with computer-based simulations. While specific microstates random, models gain precision in predicting macrostates as the size of the system grows.

Diffusion

Diffusion is the characterization of transport phenomena as a random process. Diffusion is modeled as a series of differential equations called Ficks Equations [1]. In general, modeling the movement of physical particles is characterized as diffusion.

Random Walk

The term "random walk" was coined in 1905 by Karl Pearson to describe random movement consisting of discrete steps of a fixed length [2].

The classic example in one dimension describes a drunk standing at a light pole. There is a probability p of the drunk stepping forward, and a probability of (1-p) that the drunk steps backward. The step length is always the same, and each step is mutually independent.

Random walks are used as a basis for describing many random processes, including diffusion. Applications range from particle motion to pricing stock options.

At its root, a random walk is a binomial process. In one dimension, each step provides a discrete, dichotomous forward or

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backward movement. Extending this further, the distribution has discrete displacement values that are integral multiples of the step length [3].

As the distribution increases in size (Number of steps >>0), these discrete values can be approximated as continuous, and hence random walks may be described with a Gaussian distribution [4].

Fractals

Fractals are "a rough or fragmented geometric shape that can be split into parts, each of which is (at least approximately) a reduced-size copy of the whole" [5]. The study of fractals is the subject of mathematical geometry, and fractal models are often used to describe biological diffusion.

Fractals are relevant to a discussion of diffusion as quantifying the patterns of random processes often draws from mathematical theory [6].

The mass dimension of a fractal of particles is characterized in equation (1), where n is the number of particles, r is the radius of the fractal from the starting point, and d is the mass dimension [7].

(1) $n = r^d$

Hence, in two dimensions, the upper limit of d occurs in a circle of particles, with a maximum mass dimension given in equation (2).

(2)
$$2 + 2\frac{log(\pi)}{log(r)}$$

Furthermore, in three dimensions, the upper limit of d occurs in a sphere of particles, with a maximum mass dimension

(3)
$$3 + 3\frac{log(\frac{4}{3}\pi)}{log(r)}$$

It is important to note that the upper limit of the mass dimension is not equal to the number of dimensions in the Cartesian coordinate field.

Diffusion-Limited Aggregation

Diffusion-limited aggregation is a phenomenon of the accumulation of diffusing particles undergoing a random walk [8]. The fractal patterns, called *Brownian Branches*, are known for the branch structure they form as particles become more likely to attach to a fringe particle instead of an interior portion of a branch. However, as the probability of attachment for adjacent particles decreases, the mass dimension of the fractal increases - that is, the mass dimension increases.

Literature gives the mass dimension of a 2-D simulation as 1.71, and of a 3-D simulation as 2.5 [7].

Methods

Stick Probability

In a basic DLA simulation, when a floating particle becomes adjacent to a stuck particle, the floating particle ceases its random walk and becomes stuck. This creates the classic Brownian tree clusters. However, simulations were written that allow for a variable probability that a floating particle would stick should it become adjacent to a stuck particle. We refer to this as the *stick probability*.

Mass Dimension

Mass dimension was used to compare the accuracy and precision of our DLA results with literature values. The mass dimension is a measure of how many particles aggregate in a given area relative to the seed particle. The equation (1) is used for two and three-dimensional quantitation of mass dimension. *n* is the number of particles within *r* units of the seed particle, and with *d* as the mass dimension. Thus, the mass dimension can be solved with equation (4).

$$d = \frac{log(n)}{log(r)}$$

(4)

Matlab Techniques

Zeros

Zero matrices were used in the DLA experiments. Values of zero in the matrix signified that no particle was stuck, while a value of 1 signified that a particle was stuck. The simulations begin with creating a *map* in the form of a zeros matrix, then initializing a seed by changing one of the matrix values to 1.

"Add" Factor

Matlab does not allow for negative indices in matrices. Some files contain a constant called *add* - this factor is used for translating the quadrants of a Cartesian plane to a matrix with no negative indices. In larger simulations, we chose to simplify calculations by having the seed particle be at the origin, then having the creation and kill radii be radial with respect to the origin.

However, to quantitate the sticking of a particle outside the first quadrant, we use the add factor to shift the whole plane into the first quadrant, thus allowing it to be saved in a matrix.

Example: In a 2-D simulation with boundaries 4 units from the origin, we initialize a matrix of 9 units by 9 units to represent the integral points in the plane. To input the point (0,0) in the matrix, we use an "add" factor of (1 + radius) = 5, therefore the Cartesian point (0,0) becomes the indices [0+add,0+add] = [5,5] in the matrix. Similarly, for the point (-4,-4) become [1,1] in the matrix.

Visualization

We found the Matlab function *imshow* to be the best way of visualizing a matrix in two dimensions in Matlab, per our above procedure. We have neither found nor yet created a function for the display of a matrix map of a 3-D DLA, so 3-dimensional DLA does not have a way of displaying its results visually.

Underlying Assumptions

Kill Zone Method

When considering particles undergoing a random walk, it is important to determine what happens when a particle reaches a boundary.

Choices include:
- "Bouncing" the particle back onto the simulation, effectively reversing its velocity
- Killing the particle and moving onto another one

- Having the particle re-enter the simulation from the other side

For our DLA simulations, we chose to have kill boundaries on all of our planes, so that a particle that moves out of dimensions is immediately terminated and another particle is created on the creation radius.

Procedures

Full code available at http://github.com/philipithomas/diffusion

1-D Random Walk

We simulate a 1-dimensional random walk with a variable number of steps. The displacement of multiple trials is displayed as a histogram. The step probability, number of steps, and number of trials may be modified.

2-D Random Walk

We simulate a 2-dimensional random walk with a variable number of steps. The program outputs a graph showing the path of the random walk. The probability for a step in each direction is fixed and equal for all four directions The number of steps, and number of trials may be modified.

2-D DLA

We simulate a two-dimensional diffusion limited aggregation. A seed particle is initialized at the origin. Particles are randomly initialized on a circular boundary with a corresponding circular kill zone. Stick probability may be varied.

The program runs until the aggregated particles reach the creation radius, or until a defined number of particles is created. It then outputs mass dimension and a visualization of the simulation.

3-D DLA

We simulate a three-dimensional diffusion limited aggregation. A seed particle is initialized at the origin. Particles are randomly initialized on a spherical boundary with a corresponding spherical kill zone. Stick probability may be varied.

The program runs until the aggregated particles reach the creation radius, or until a defined number of particles is created. It then outputs mass dimension.

Results

1-D Random Walk

For the 1-dimensional random walk simulation we measured the displacement of a particle undergoing a random walk originating at the origin for a given number of steps. A histogram was constructed that shows the number of times a certain displacement was recorded after a given number of trials. For an equal probability of stepping left or right (p=q= 0.5), the histogram can be approximated as a normal distribution with the mean located near the origin. Making a particular direction more probable by changing the value of p causes the histogram to shift toward that side. For the large scale experiment, the mean displacement and standard deviation was calculated for 1,000 trials of a 1,000 step random walk for p = 0 to p = 1 in 0.1 increments. From the mean and standard

deviation, we were able to plot the normal distributions in Figure 2. The distributions matched closely to the expected distributions that were calculated from p and n (Table 1) .

Table 1: Comparison of trial data to expected data for a Gaussian distribution for varied p probabilities

| p	Actual µ Displacement	Actual σ	Expected µ Displacement	Expected σ	Percent Error of Displacement	Percent Error of Standard Deviation
0	-1000	0	-1000	0	0.00%	Undefined
0.1	-798.958	19.532	-800	18.97366596	0.13%	-2.94%
0.2	-600.528	25.3496	-600	25.29822128	-0.09%	-0.20%
0.3	-398.868	30.1053	-400	28.98275349	0.28%	-3.87%
0.4	-198.75	31.7441	-200	30.98386677	0.63%	-2.45%
0.5	-1.636	32.6863	0	31.6227766	Undefined	-3.36%
0.6	200.184	30.2768	200	30.98386677	-0.09%	2.28%
0.7	398.636	28.6368	400	28.98275349	0.34%	1.19%
0.8	599.184	25.2495	600	25.29822128	0.14%	0.19%
0.9	800.114	20.2459	800	18.97366596	-0.01%	-6.71%
1	1000	0	1000	0	0.00%	Undefined

Random walk in 1 d with probability p =0.5 with100 trials and50 steps
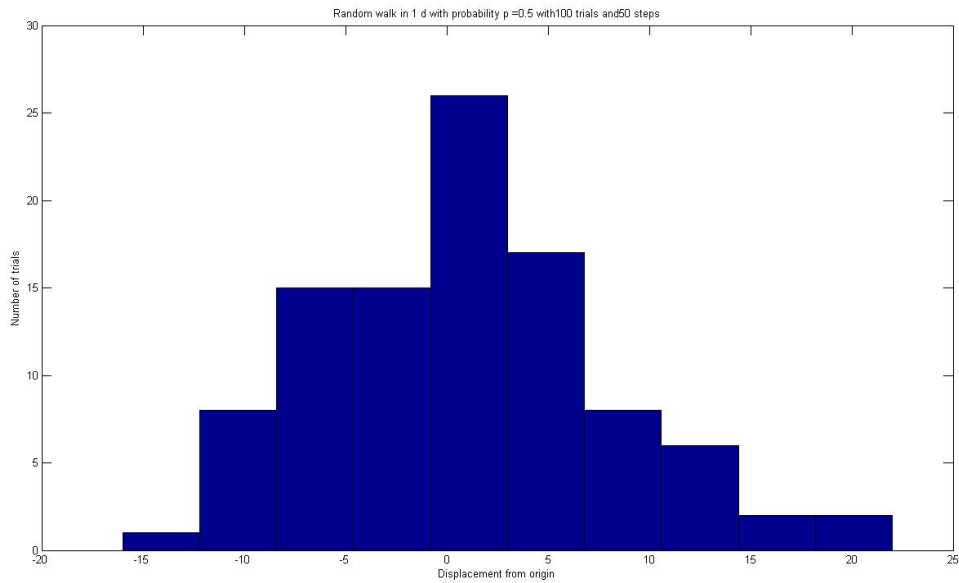
Figure 1: Histogram of 100 trials of a 50 step 1-D random walk.
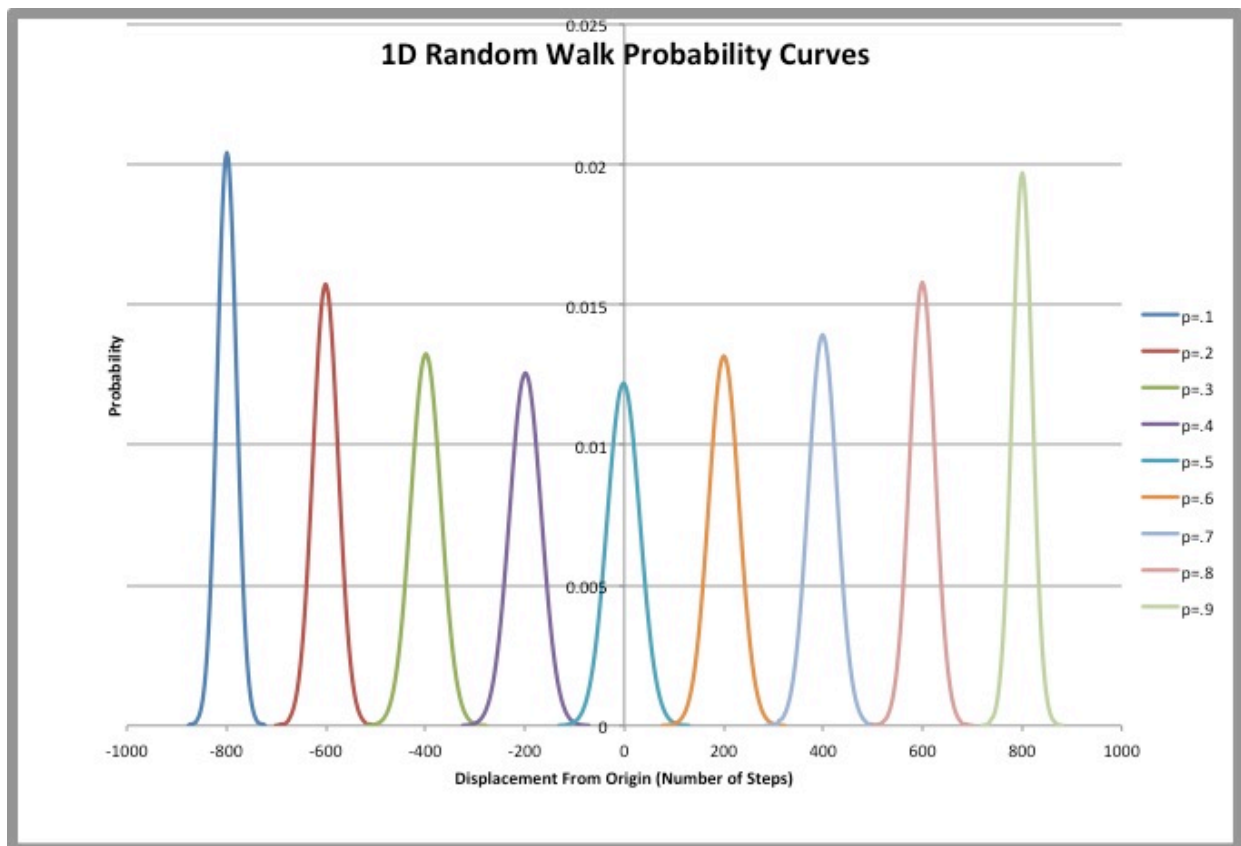

1D Random Walk Probability Curves

Figure 2: Normal plots based on mean displacement and standard deviation for 1,000 trials of a 1000 step 1D Random Walk at a given probability p to take a step

2D Random Walk

Our program simulated 1000 trials of a 1000 step 2-dimensional random walk. The average displacement from the origin was 0.5533 units. We were also able to plot the path of the 2D random walk. A red marker is placed at the common origin and a black circle marks the ending point of each trial.

Multiple trials were plotted on one graph, with each color corresponding to a different random walk.
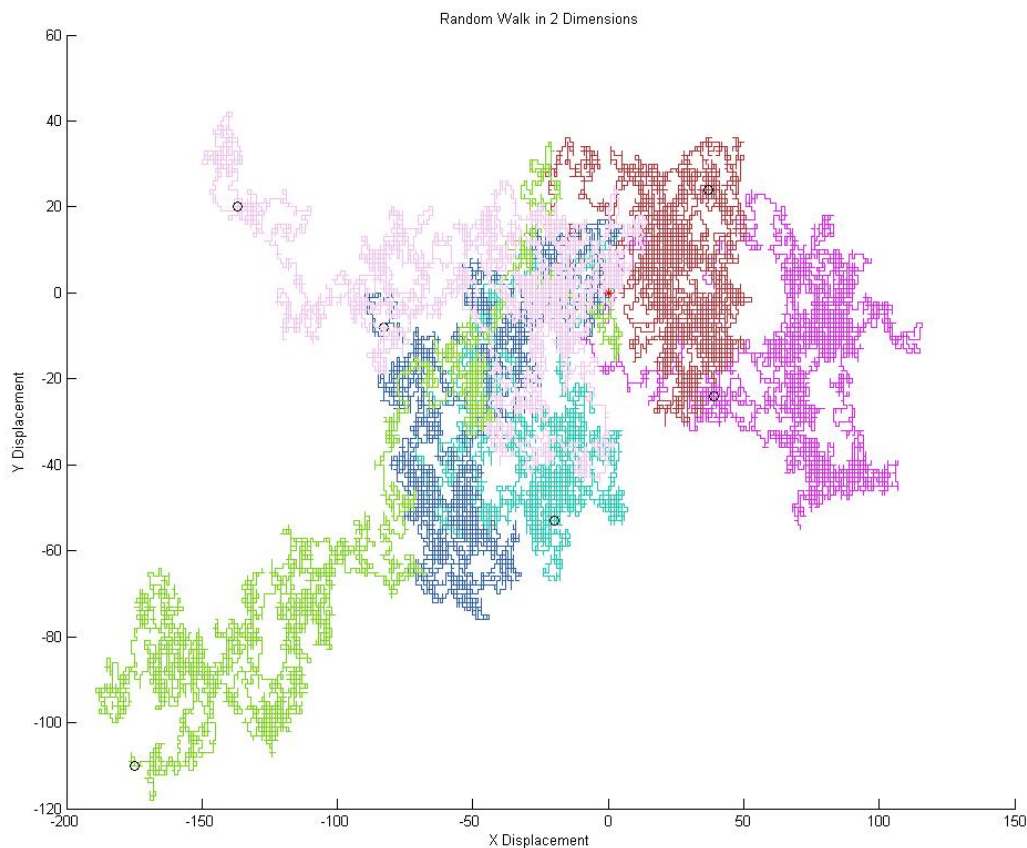
Figure 3: Six trials of a 2-D random walk of 1,000 steps each. The red asterisk marks the origin for all trials, and the open circles mark the final displacement of each particle

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DLA

The output of the 2-dimension DLA simulation yields a cluster with a branched, outward growing structure as shown in figures 4-8. The reason for the branching structure is that it is difficult for a random walking particle to reach the interior since it must avoid the branching walls or else it will get stuck and start a new branch. The mass dimension is measured from two simulations with varying radii. The smaller simulation (Figure 4) has a radius of 83.863 units with 2,436 stuck particles. We use equation 4 to find that the mass dimension is 1.7606. The larger simulation (Figure 5) has a radius of 834.101 units with 122,797 stuck particles .The mass dimension is 1.7421. These values are very close to the literature value of 1.71 as determined by Witten and Sander. [8]
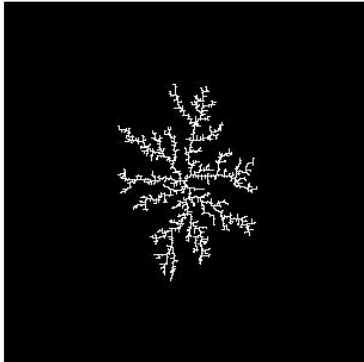
DLA with Stickiness

Changing the probability that a particle would stick when adjacent to a stuck particle had a significant effect to appearance of the clusters, and consequently to the calculated mass dimensions. By decreasing the sticking coefficient, it is now less difficult for a random walker to move between the branches. It can hit a branch without necessarily getting stuck and can diffuse deeper towards the interior. This results in the higher density clusters as shown in figures 6-8.

The effect of the sticking coefficient on mass dimension is demonstrated in Figure 9. Plotting mass dimension as function of sticking coefficient gives a logarithmic curve.
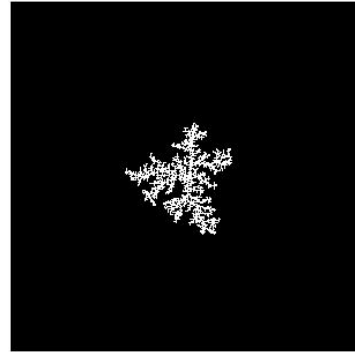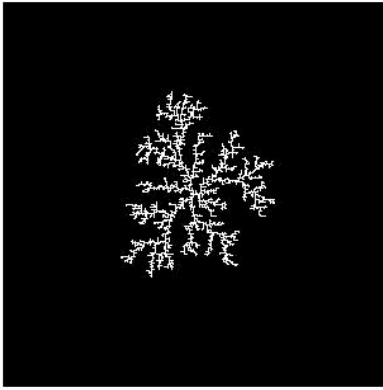

Figure 4: 2-D DLA cluster with ~2500 particles. d=1.706.

Figure 5: 2-D DLA cluster with ~120,000 particles. d=1.74.

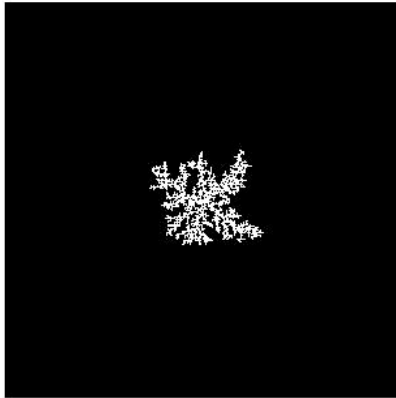**Figure 6: DLA cluster with stick coefficient = .5. d=1.798.**

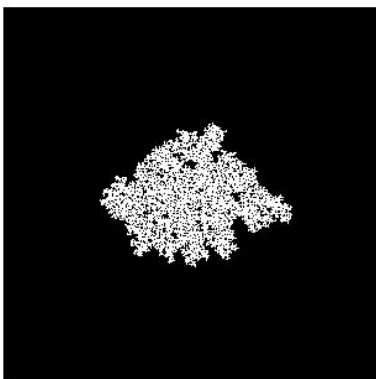**Figure 7: DLA cluster with stick coefficient = 0.1. d=1.909.**

Figure 8: DLA cluster with stick coefficient = 0.01. d=2.011

3-D DLA

The mass dimension values for the 3-dimension DLA simulation ranged from d=2.18 for a stick coefficient of 1, to d=2.50 for a stick coefficient 0.1. The results are plotted in Figure 10. Our results do precisely match the literature value for the mass dimension for a stick coefficient of 1 (d=2.5). This may be attributed to memory constraints using Matlab since we had to decrease the radius in order for the program to run. However, mass dimension values do increase as the stick probability decreases as expected.

Discussion

Applicability to life systems

Diffusion-limited aggregation can be used simulate the types of branching clusters that resemble physical processes and objects in real life. Examples include electrodeposition and dielectric breakdown. Electrodeposition is a process by which an electrode is coated by metal ions in a solution that diffuse by an electric field. To obtain DLA clusters similar to those created by our simulation, a circular anode is used to surround the solution and a cathode is placed at the center to serve as the seed. Running an electric current will cause the metal ions to diffuse from the cathode through the solution and deposit onto the anode at the center. Increasing the voltage will result in a more dense structure. This is because the anode attracts the ions more strongly and as a result the probability that the ion will stick to a branch decreases. [9] Matsushita et al. measured mass dimension of the electrodeposition of zinc ion at different voltages and found that as voltage

increased from a threshold voltage, mass dimension increased linearly from about d=1.66, the approximately the value for a sticking coefficient of 1, to about d=1.85, the value we observed for a sticking coefficient between 0.1 and 0.2. [10]. In another study by Brady and Ball, the mass dimension of copper electrodeposits was measured, which resulted in a 3-dimensional DLA aggregate with a d=2.43.

Dielectric breakdown also exhibits a DLA-like structure. When an insulating material is exposed to a strong enough electric field, conducting pathways form through the insulating material. One example is lightning, in which intense electric fields form a pathway through the air.

Randomness of computers

One concern regarding computer simulations of diffusion and random walks is the whether the random number generator can output a suitably random number for the particular task. The rand function in Matlab is a pseudorandom generator that uses an algorithm based on a hash of the unix timestamp to generate numbers. True randomness can be achieved in computers using devices that replicate a 2-slit experiment, thus generating 1 and 0 outputs with quantum mechanical phenomena.

While not truly random, the Matlab-generated random numbers used in our experiment are used, at most, to randomize a decision from four choices. The random function is sufficiently evenly distributed over four quadrants that the error is negligible.

Possible extensions

Our random walk program is a simple model to simulate the movement of a single particle in Brownian motion. A possible extension is to simulate the movement of multiple particles at one time. The DLA program we use introduces only one particle at time, and no new particle is introduced until the current particle sticks or exits the boundary where the time (measured in number of steps) of the random walk can vary. Using multiple particles may more closely approximate reality in which these particles can interact with each other.
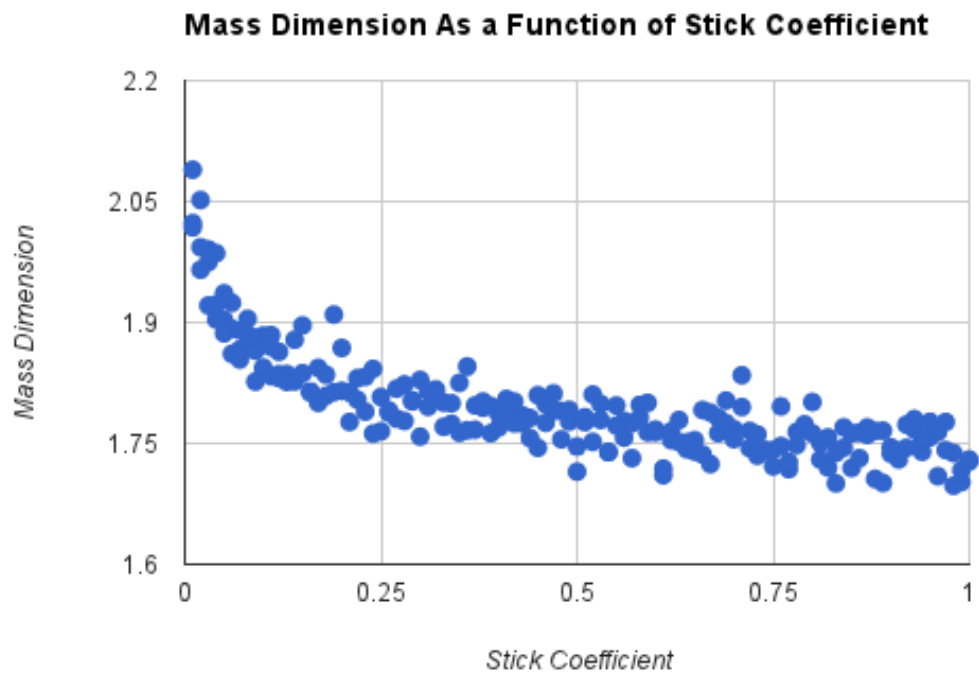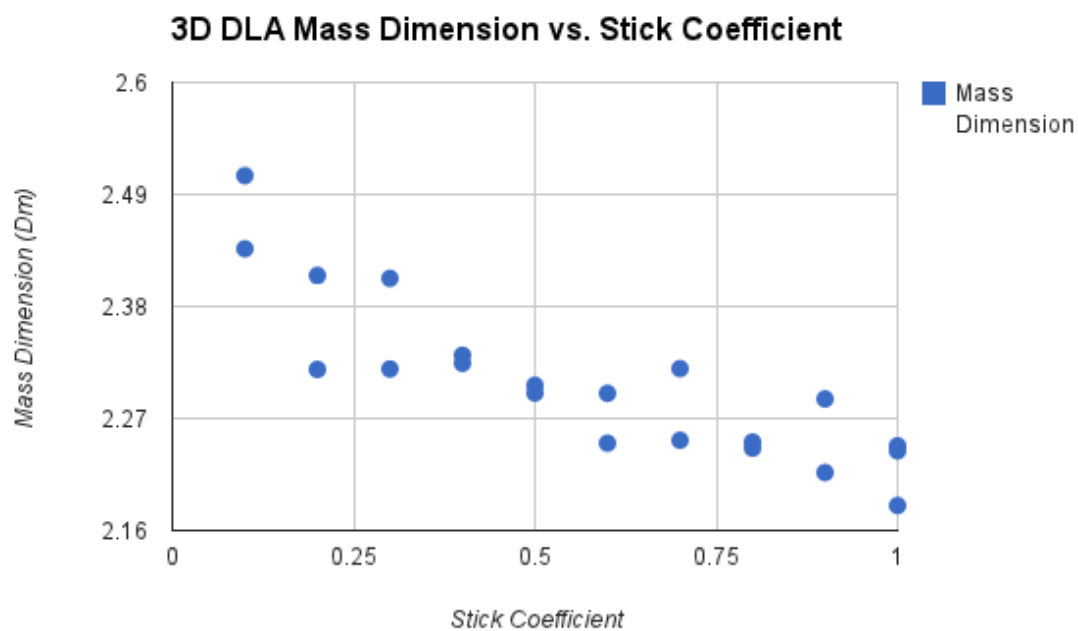
Mass Dimension As a Function of Stick Coefficient

Figure 9: 2-D DLA mass dimension as a function of stick coefficient from 0.01 to 1 in 0.01 increments for three radii (83, 209,

3D DLA Mass Dimension vs. Stick Coefficient

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Figure 10: 3-D DLA mass dimension as a function of stick coefficient from 0.1 to 1 in 0.1 increments for 2 trials of radius = 125.

Sources

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