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Effect of Starting Location on Clusters Formed by Diffusion-Limited Aggregation

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Abstract

This study examines the effect of the starting location on particles that undergo diffusion-limited aggregation. Proposed in 1981 by T.A. Witten Jr. and L.M. Sander, diffusion-limited aggregation (DLA) is one of the primary models of diffusion. DLA is a growth process in which particles form a cluster by undergoing a random walk and attaching themselves one-by-one to the cluster, which is initialized by a central seed particle. This model of diffusion explains many patterns occurring in nature, such as coral growth, dielectric breakdown, electro-deposition and others. Frequently when DLA is modeled computationally, the particle's starting location prior its random walk is on the perimeter of a circle, with a radius that is larger than the size of the cluster. However, what has been studied less is selecting a random unoccupied point for the starting location of the particle, including points within the perimeter of the cluster. To examine the effects of the different starting locations, we have created a two-dimensional off-lattice computational simulation of DLA. By using measurements such as radius of gyration, fractal dimension and lacunarity, we can characterize and compare the clusters formed. Since research on DLA is heavily reliant on computational models and simulations, our results could shed light on whether the starting locations of the particles need to be more explicitly considered for certain physical examples of DLA.

Keywords: Diffusion-limited Aggregation, Starting Location, Cluster Growth

1. Introduction

Diffusion of particles is one of the major components of transport phenomena, and one of the primary models of it is diffusion-limited aggregation[1] (DLA). In the most common model of DLA, a seed is fixed at the center of a region and then a particle is released from a random location around the perimeter of a circle outside the cluster. The particle undergoes a random walk until it either has to restart, since it walked out of the allowed region, or it hits the seed and irreversibly sticks. Then another particle is released, and undergoes the same process. The results of this model show very fractal-like aggregates, as shown in Figure 1. One of the reasons DLA is of great interest to the physics community is because although the model has simple rules, it produces clusters that mimic complex natural phenomena even when the physical processes are very different[2]. For example, although the processes of dielectric breakdown and coral growth are obviously different the overall growth pattern is similar. Currently, there is no complete theoretical model that explains DLA[3]. DLA is studied both computationally and experimentally, although more frequently the former. Large-scale computational studies are typically used, however those are extremely computationally expensive thus difficult to create.

In an attempt to add to the overall understanding of DLA, this particular study explores the effect of the starting location of the particle prior to the random walk. This is done at a moderate scale, with the maximum cluster size of 10^6 particles. In the random start model, rather than releasing the particle from a point outside the cluster, the

particle is allowed to start from any unoccupied point in the region. This has not been explored extensively, and currently the common model is used for a variety of different physical processes.

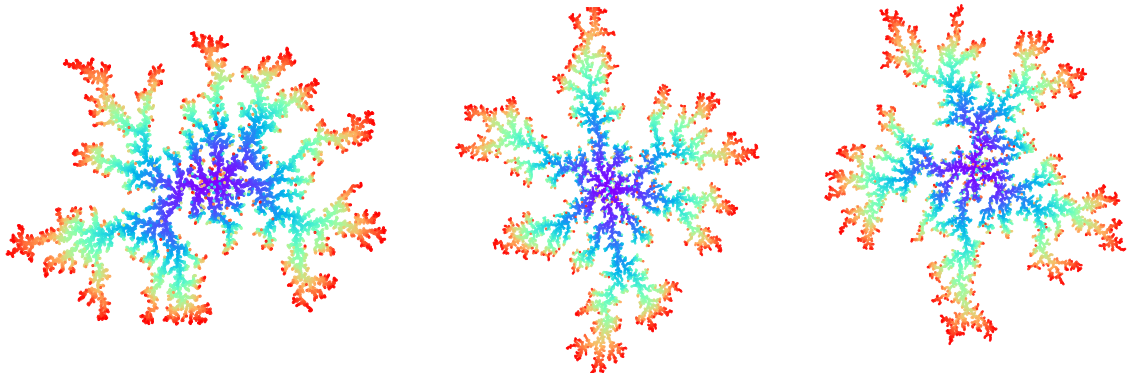

Figure 1. Three clusters produced by our simulation program; colors show the evolution of the cluster with respect to time. Particle size is exaggerated for aesthetics; there is no actual overlap.

There are several well-known parameters that can affect the general structure of the DLA cluster, such as the size of the step the particle takes during its random walk and the total number of particles[4]. In order to fully investigate the effects of the starting point models, it is necessary to use various step sizes and number of particles. This paper shows how the random starting location affects the growth of the cluster when compared to the common model. The proceeding sections explain the two different starting locations, discuss the computational techniques and basic algorithms used, describe the calculations used to characterize the cluster, and then present the results.

2. Methodology

2.1. Starting Locations

The most frequently used starting location for particles undergoing DLA is outside the cluster, which this study refers to as the common model. In the common model, a particle's initial location is randomly selected around the perimeter of a circle (outside the maximum radius of the cluster), and then it begins its random walk only stopping when it collides with a particle in the cluster. If the particle walks outside the allowed region it is restarted at a new random location on the perimeter of the circle. Once that particle joins the cluster, another one would be released from the perimeter of the circle and undergoes the same process.

In the random starting location model, a particle can start at any unoccupied point, including points within the cluster. There is still a center seed in the same location as the common model, and the particles undergo the random walk with the same basic parameters as the common model. Typically with the common model most of the particles aggregate towards the end of the branches, since that is the more likely location for the particle to stick. For the random start model however, the initial predictions were that it would produce denser clusters; since the particles are able to start inside the cluster and stick in locations statistically they would not with the common model. This idea is elaborated on in Section 3.

2.2. Computational Simulation Algorithm

In order to explore the effects of starting location we created a two-dimensional, off-lattice computational simulation of DLA using C++. In the program, the particles were represented as solid disks with a radius of one unit. All distances were measured in these units. The size of the universe (where the particles were allowed to walk) increased as the total number of particles in the clusters increased in order to prevent edge effects. To create a more efficient and faster program, a grid with cells significantly larger than a single particle was added. Therefore, as the particle diffused and aggregated it was assigned to the grid cell containing its current location. The overall algorithm for both models is described in Figure 2, which only applies to particles that are close to the cluster. When the

particles are far from the cluster they take much larger steps in order to speed up the program. Also, when the particles walk beyond the edge of the defined universe they are restarted as new particles.

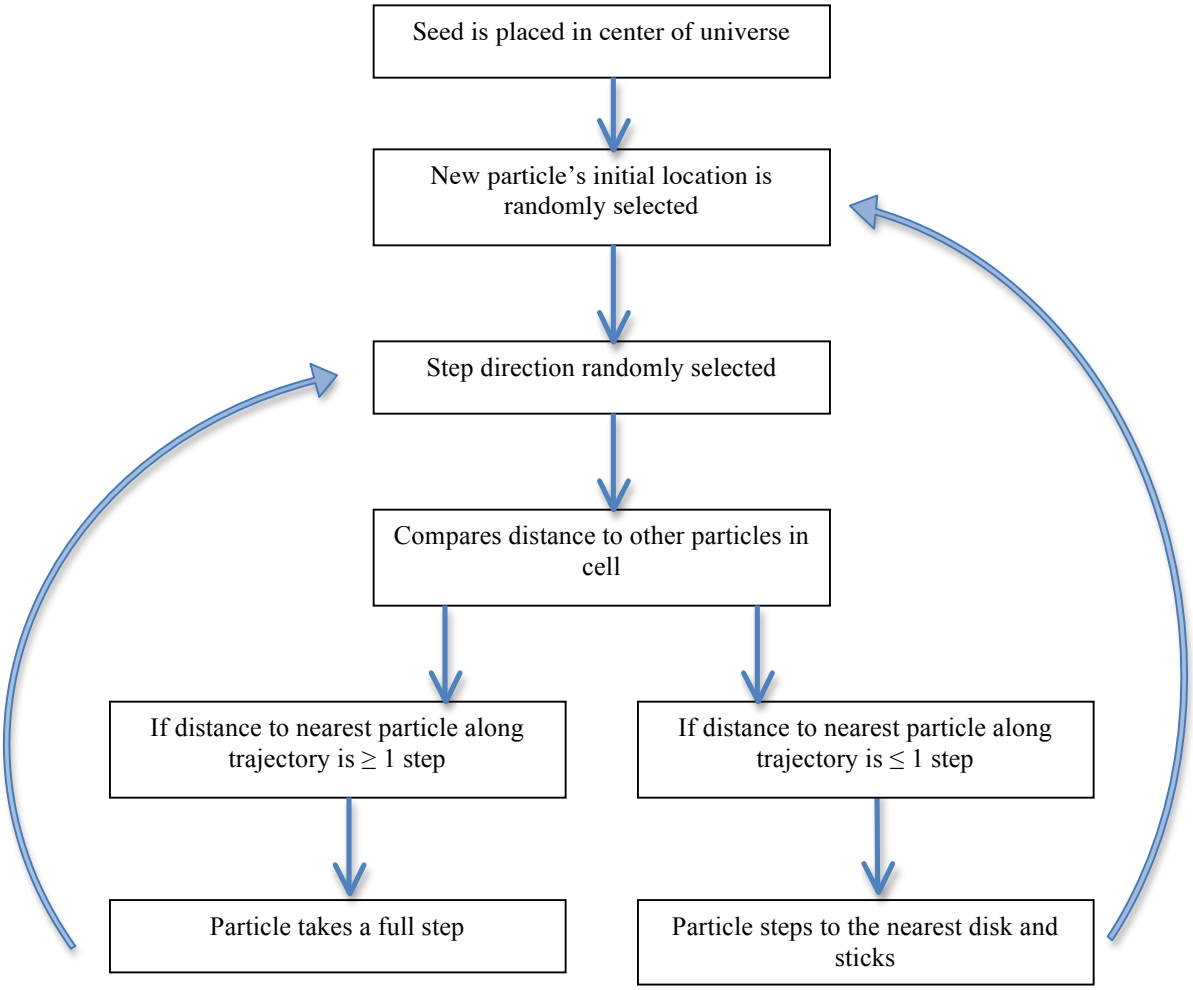

Figure 2. Algorithm flow chart for our simulation program

2.3. Characterizing the Clusters

In order to characterize and compare the clusters we used three measurements: radius of gyration, fractal dimension, and lacunarity. Radius of gyration (R_g), which is shown in equation (1), is the average distance between every stuck particle and the seed and is an overall measure of compactness.

$$R_g = \sqrt{\frac{1}{N}\sum (R_{particle} - R_{seed})^2} \quad (1)$$

N is the total number of particles, and $R_{particle}$ - R_{seed} is the distance from a given particle to the seed. Radius of gyration is frequently used in studies on DLA, and is especially appropriate for this study since it was anticipated that the random starting location would produce more compact clusters. Radius of gyration is also used to find the fractal dimension of the cluster[5], which can be found using equations (2) and (3).

$$R_g \sim N^{\beta} \tag{2}$$

$$D = \frac{1}{\beta} \tag{3}$$

In equation (3) D is the fractal dimension, more specifically the Hausdorff dimension. By finding the fractal dimension, it was possible to determine if the random starting location affected the fractal nature of the cluster.

Lacunarity is a measure of how evenly the particles are distributed[6]. Clusters can have the same radius of gyration, but have a very different arrangement of particles. So lacunarity is a valuable measurement since it is able to account for some of those possible differences. To determine lacunarity, a particle is selected as the center of a circular box and the number of particle centers in the box (n) are counted – this is then repeated over the cluster. This is known as the sand box method[7]. The average of n is the first moment, $Z^{(1)}$, as described in equation (4). The second moment, $Z^{(2)}$, is defined in equation (5) and the lacunarity, Λ, is defined in equation (6).

$$Z^{(1)} = \langle n \rangle \tag{4}$$

$$Z^{(2)} = \langle n^2 \rangle \tag{5}$$

$$\Lambda = \frac{Z^{(2)}}{[Z^{(1)}]^2} \tag{6}$$

In order to capture the self-similar nature of the cluster, it would be ideal to only perform these calculations on a single branch of the cluster. However, since that is logistically difficult, an easier method suggested by Hanan and Heffernan[8] was to perform the lacunarity calculations in a annulus region of the cluster as shown in Figure 3. By excluding the tips of the branches and the center region, it gives approximately the same results as if only using a single branch.

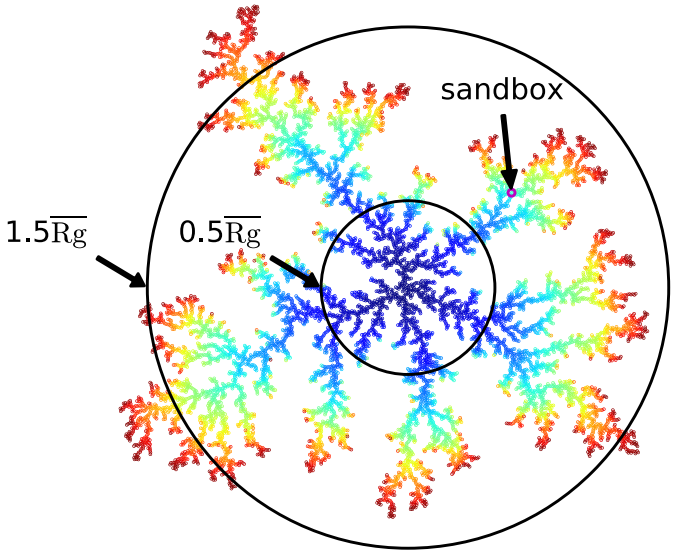

Figure 3. Pictorial representation of the annulus used for the sand box method.

As Figure 3 shows, the inner circle of the annulus has a radius of 0.5 times the average radius of gyration (determined over multiple trials), and the outer circle has a radius of 1.5 times the average radius of gyration. The object labeled "sandbox" in Figure 3 is an example of a single box used for the lacunarity calculations. In the following analysis, the box radius size used was 0.02 times the average radius of gyration.

3. Analysis

Trials were simulated for each starting location model using step sizes (as a multiple of particle radius) 2^1, 2^2, 2^3, 2^4, 2^5, 2^6 in combinations with 10^2, 10^3, 10^4, 10^5, 10^6 particles. Forty clusters were generated for each trial. The first results were simply pictorial results, and samples of two clusters are shown in Figure 4.

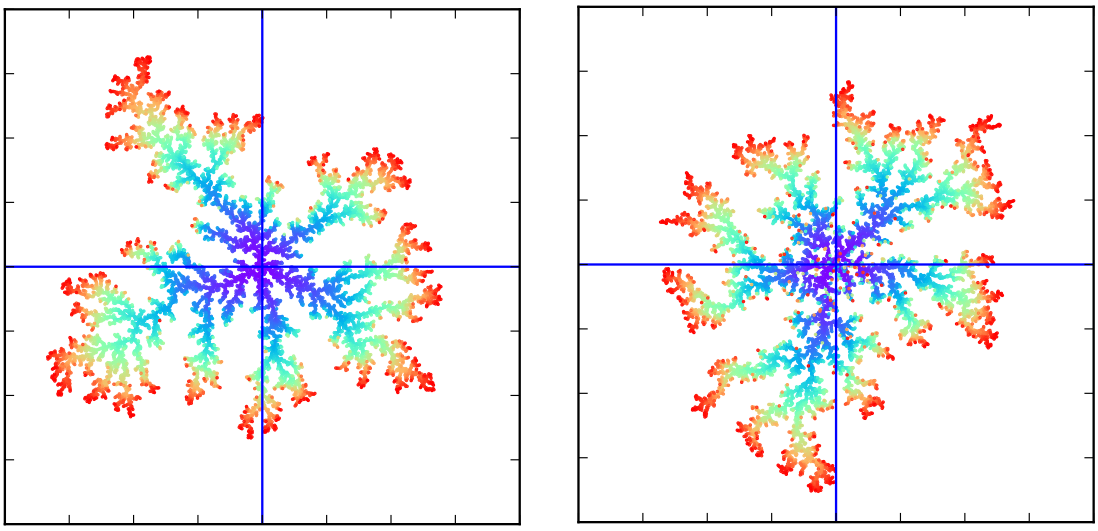

Figure 4. On the left is a cluster formed by the common model, and on the right is a cluster formed by the random starting location. Both clusters have 10^5 particles and a step size of 2.

The colors are an indication of the time evolution of the cluster, with the cool colors representing particles that aggregated earlier in the program, and the warm colors representing particles aggregating later. As evident in Figure 4, the clusters formed by the random start model have a significant number of warm-colored particles close to the center of the cluster and within the branches, a trend not observed in the clusters formed by the common model. This means that the overall growth of the clusters using the two models do produce different clusters, at least visually. The following sections elaborate on this trend using the quantitative measurements discussed in Section 2.3.

3.1. Average Radius of Gyration

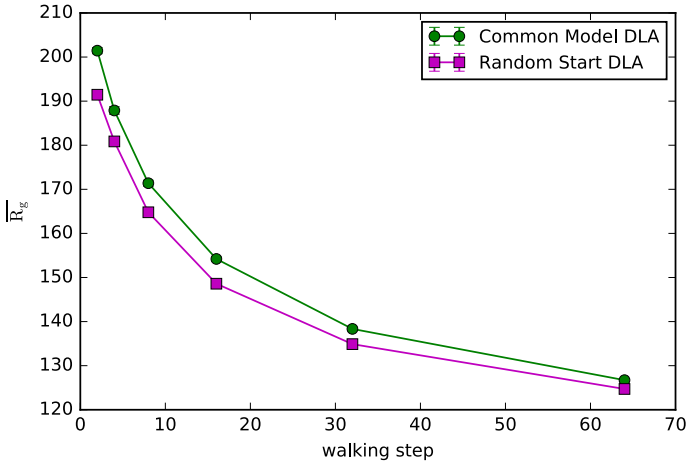

Figure 5. Graph of the average radius of gyration with respect to step size for both models, for 10^4 particles; each symbol is larger than an error bar

As anticipated, the random start model produced a consistently more compact cluster than the common model as shown in Figure 5. However, the random start model only produced results like those in Figure 5 for cluster sizes 10^4 and above. For the smaller clusters, the radius of gyration was approximately the same for both models. This discrepancy was expected; many trends of DLA can be observed only for larger cluster sizes.

3.2. Fractal Dimension

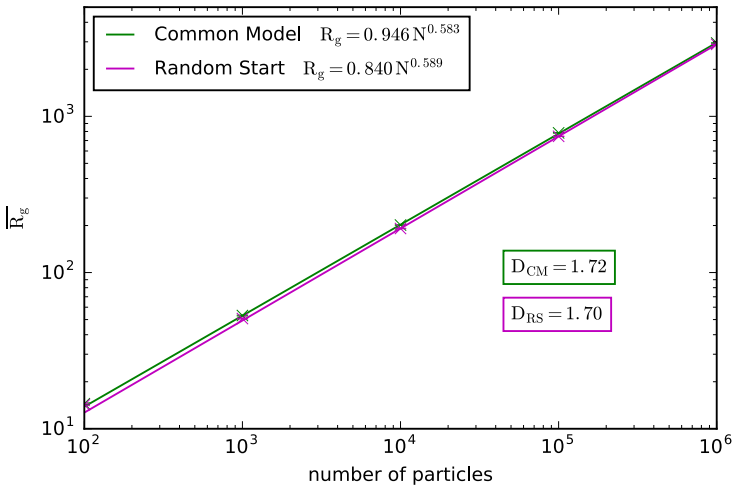

Figure 6. Log-log plot of the average R_g versus the number of particles with a power law fit

The log-log plot shown in Figure 6 was used to find the power law relationship as described in equation (2). Using equation (3), the fractal dimensions for the common model (D_{CM}) and the random starting location (D_{RS}) are determined by taking the reciprocal of the slope shown in Figure 6. These results show that both starting locations have essentially the same fractal dimension. The most accepted value[9] for the fractal dimension of DLA is around 1.71, so overall these results showed that the random starting location did not affect the fractal nature of DLA.

3.3. Lacunarity

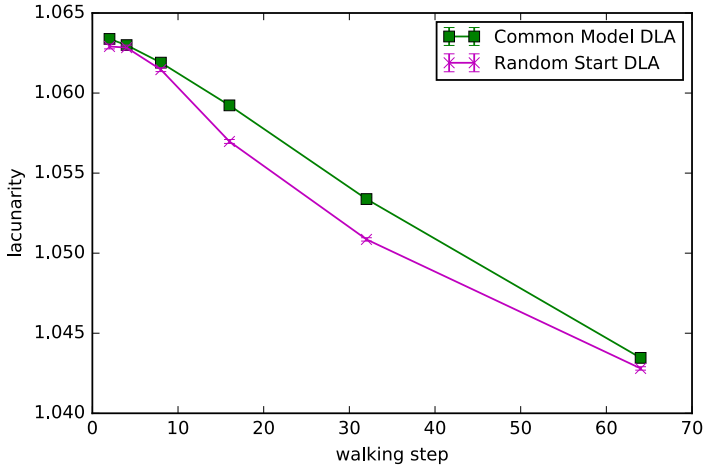

Figure 7. Graph of the lacunarity with respect to step size for both models, for 10^6 particles

The graph in Figure 7 shows that the random starting location produces less lacunar, more evenly distributed clusters. These values are also statistically significant; each of the symbols is about the size of an error bar. However, similar to the results from the radius of gyration, the distinct differences between the models like in Figure 7 were only observed for large cluster sizes. As the cluster size decreases, the difference in lacunarity decreased as well.

4. Conclusion

This study was able to show that the random starting location does affect the growth of the cluster formed by DLA by creating more compact and more evenly distributed clusters. However, larger clusters will need to be analyzed to see if the trends continue for radius of gyration and lacunarity. The main problem with creating larger clusters is the amount of computational effort and time it takes. Some options to allow for the creation of larger clusters include: modifying the algorithm, improving the hardware and possibly using parallel computing.

Also, to further understand the lacunarity results more tests should be done to see how the box radius used in the sand box method affects the results. Specifically, to see if the random start model consistently produces less lacunar clusters. The tests could include using the same box radius for all cluster sizes, and using a wider variety of box radii for a single trial.

The next step would be to look into what physical applications, if any, the random start model actually represents. By exploring the physical representations it would be easier to determine what calculations and measurements would more completely reflect the differences in growth.

5. Acknowledgments

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6. References

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