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CBE 641 – Transport Processes

Final Project

Diffusion-Limited Aggregation and the effects of local particle drift and sticking probability on the fractal dimension of a cluster

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Abstract

A computer model of a diffusion-limited aggregation cluster grown in a 2-dimensional lattice was generated as a base case to analyze the behavior of such clusters and their fractal dimension (calculated via two different methods). The effects of a local particle drift probability and a sticking probability on fractal dimension were investigated, as well as a variation from the base case where clusters are grown inwards from an initial circle with fixed radius. It was found that the fractal dimension of a cluster in the base case falls within the expected range of values ($D_f \approx 1.71 - 1.77$) that has been found theoretically and in previous published studies. When applying a drift to each particle in the system, the clusters grow in the direction opposite to such drift and their fractal dimension increases as the drift probability increases. In addition, when considering a particle does not always stick to the first adjacent point in the cluster, lowering the probability that it does stick results in an increase of the fractal dimension. This behavior has also been observed in previous studies.

I. Introduction

Diffusion-limited aggregation (DLA) is a process in which individual particles perform random walks and cluster together to form a main aggregate of such particles. In principle, the process is initiated by a single particle to which many other particles are aggregated, one by one, in order to ultimately form a single cluster. This process was proposed in 1981 by Witten and Sander [1], who developed a model for cluster growth controlled by a random diffusion process. This model, along with many of its variations that have been developed since, is applicable for systems in which diffusion is the main transport method for the particles.

The aggregates that result from DLA are examples of fractals. Fractals are generally defined as complex self-similar structures that are created by continuously repeating a process (DLA in this case). Fractals are important and interesting irregular structures because they are found in a broad range of areas in nature, such as the growth of roots, snowflakes, corals, broccoli, lightning paths, and many others. A very important parameter that has been widely studied in order to characterize such shapes is the fractal dimension. This parameter relates the number of particles in a cluster to its size and, according to theory and previous studies, it can be found to be approximately 1.71 – 1.77 when a cluster is grown in a 2-dimensional lattice.

One of the leading methods of studying the behavior of these DLA structures is through computer simulations. In this study, a MATLAB code was used to analyze a DLA cluster as well as DLA clusters with additional parameters, such as a "sticking" probability and a drift probability.

II. Methods

A DLA cluster was first generated on a two-dimensional lattice (x vs. y, square matrix in MATLAB). The algorithm for this process consists of initially occupying the center of the lattice with a single particle and individually aggregating particles to achieve a final, bigger cluster. An aggregated particle is simulated by a '1' in the square matrix, with all other sites being '0'. The radial position is calculated by $R = \sqrt{x^2 + y^2}$ and rounded to index a point in the matrix. Each particle is occupied at a radius slightly larger (R_s) than the radius of the cluster (R_{max}) and with a random direction. The particle then performs a random walk until it comes into proximity with the cluster and aggregates to it. This process is simulated in the code by first moving the particle to a randomly selected adjacent site ($x \pm 1, y \pm 1$). A function '*check*' is then called after every move to determine the state of the particle. If there is a particle from the cluster adjacent to the moving one, the algorithm will aggregate the latter to the cluster and proceed to occupy and move the next one. If there is no adjacent occupied site, the particle will continue being moved. A radius limit (R_{kill}) was also set so that, if the particle exceeds such position, it will be 'removed' and a new particle will be occupied and moved. This is done to avoid a particle from moving extremely far from the cluster and never coming back, causing the algorithm to never end. In addition, a function '*circlejump*' was incorporated to accelerate the algorithm. The '*check*' function calls '*circlejump*' when the particle reaches a position far from the cluster but still smaller than R_{kill}. This function moves the particle by a distance ($R - R_s$) and a random direction so that it can move faster while still executing a random process. The occupied sites in the matrix were plotted to show the final cluster.

The mass of DLA fractals is generally known to scale as $m \sim (size)^{D_f}$. For purposes of this model, the mass can be considered to be the number of particles (N) in the cluster and the size to be its radius. Two methods were used to calculate the fractal dimension of the cluster from this model: **M1)** Relating N and R_{max} of the final cluster by $D_f = \frac{\ln(N)}{\ln(R_{max})}$, and **M2)** Plotting ln (N) vs. ln (R_{max}) as the cluster is growing, for which the slope of the plot is the fractal dimension.

Based on theory and previous studies, a 2-dimensional DLA fractal should have a $D_f \approx 1.71 - 1.77$.

A drift analysis was done on the DLA algorithm where a new parameter P_{drift} was introduced. When moving each particle throughout the lattice, a random number from 0 – 1 is first generated. If this number is greater than P_{drift}, the particle is moved randomly as with the original algorithm. However, if it is equal or lower than P_{drift}, the particle will be moved in one determined direction. The value of P_{drift} is varied in this study and it is expected that a drift on the particles results in a fractal growing in the direction opposite to the drift.

An additional analysis was performed where, instead of growing a cluster from the center of a square lattice, clusters were grown inwards from a circle of set radius by occupying each new particle at the center of such circle. The algorithm for this model is very similar to that for DLA, however some of the conditions are reversed (as is the model). The value of R_{kill} is that of the initial circle, and R_{max} decreases as the clusters increase in size. In addition, a new parameter P_{stick} was introduced which determines the probability of a particle sticking to the cluster when it is adjacent to such. In the original DLA model, this value was assumed to be 1. The value of P_{stick} is varied in this study and it is expected that the fractal dimension increases when lowering P_{stick}, since the particles are more likely to explore smaller areas between the long arms of the cluster. The fractal dimension in this case was determined by first calculating the area covered by the particles based on the initial radius minus the new R_{max}. A new radius was then calculated based on this area, which was used to calculate D_f by M1.

The standard error of each calculated value was calculated based on 10 runs for each algorithm. The equation used to calculate error is the following, $\varepsilon = \frac{\sigma}{\sqrt{n}}$, where σ is the standard deviation of the set and n is the number of runs considered.

III. Results and Discussion

i) DLA base case algorithm

An example of the resulting cluster from the original DLA algorithm (base case) is shown in Figure 1, for which the code was ran until 3000 particles were aggregated. The color scheme illustrates the order in which particles were aggregated, with dark blue being the first. The fractal dimension of a cluster with this number of particles was found to be $D_f = 1.743 \pm 0.006$ by using

M1 (method 1) for calculating this parameter. When using M2 (method 2), as shown in Figure 2, the slope of the *log(N)* vs. *log(< R >)* plot was found to be D_f = 1.723 ± 0.014.

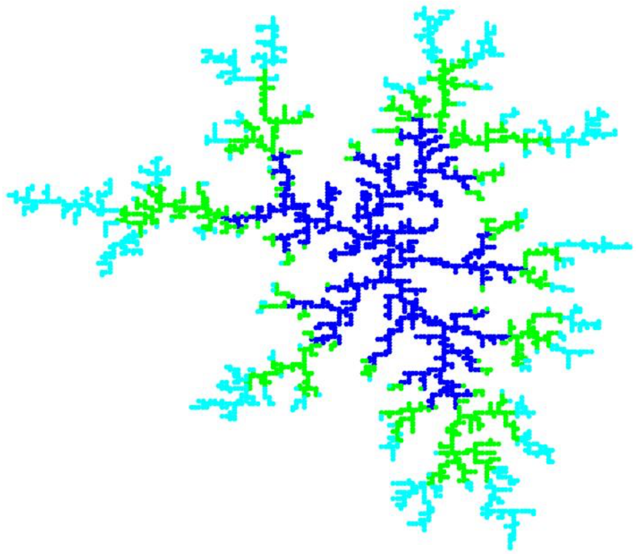


Figure 1. *DLA cluster with N = 3000 particles, Df = 1.743 ± 0.006 (M1)*

Both methods resulted in a good estimate for the D_f of a 2-dimensional DLA fractal since, based on previous models using a similar algorithm, D_f has been found to be in the range of ~ 1.71 – 1.77. However, it should be noted that M1 resulted in much more consistent values in that range while M2 resulted in fractal dimension values of as low as 1.60 at times. This is why its error is more than twice that of M1. A main source of error for this method is likely the points taken at very small radius values of the cluster. As shown in Figure 2, the *N* values for low *R* are not as steady as values after a certain radius (*log(R)* ~ 0.6). In addition, the *N* values for low *R* were very inconsistent throughout the various runs thus the higher deviations from the mean. When the code was ran for a lower amount of particles, such as 1000 – 1500, M2 resulted in even higher error values since each run resulted in very different values for the slope of *log(N)* vs. *log(< R >)*. Therefore, it is necessary to run for a very high number of particles in order to get an accurate result with M2, while M1 was much more consistent in the desired range even for smaller numbers of particles. Another source of error that affects both methods is that of the radius approximation in a square lattice, since the values of *R* are always rounded. Due to the higher error for M2 and only ~ 0.02 difference between the mean values of the two methods, M1 was used for all further analyses in this study to calculate the fractal dimension.

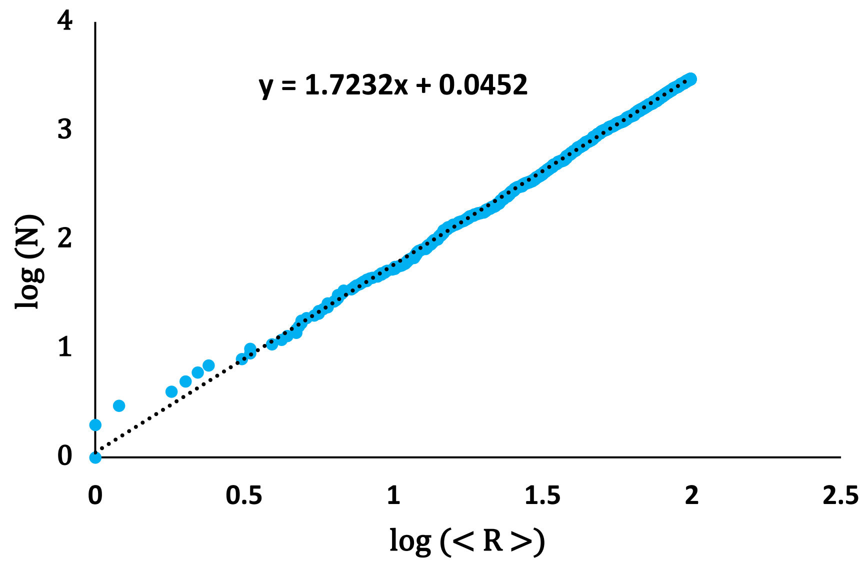
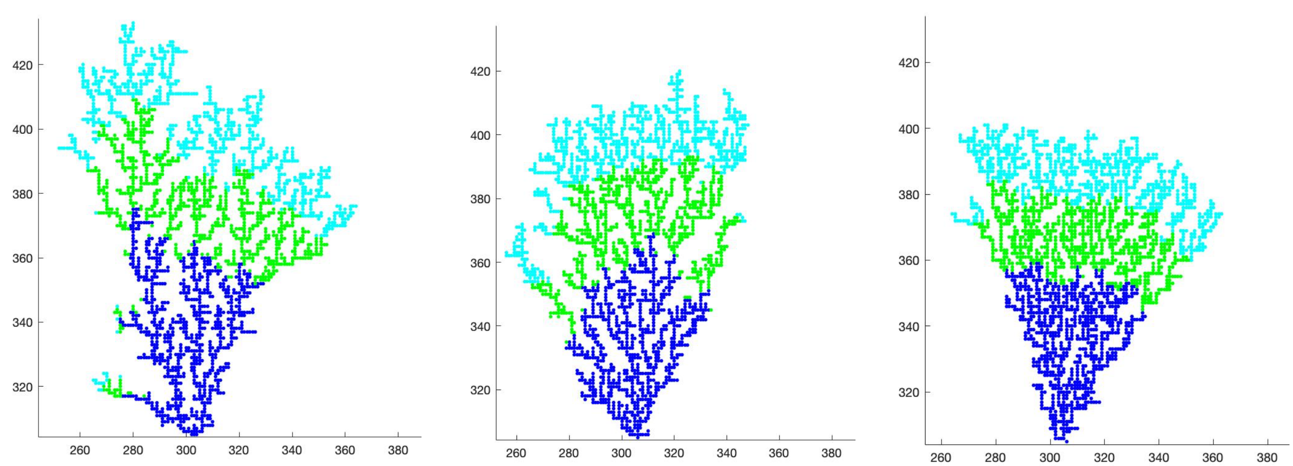


Figure 2. *Fractal dimension mass vs. radius (M2) analysis for a DLA cluster with $N = 3000$ particles, $D_f = 1.723 \pm 0.014$*

ii) Particle drift analysis

The effects of a drift probability on each particle occupied in the lattice was analyzed by forming clusters containing 2500 particles with $P_{drift} = 0.1$, 0.5, and 1. The final cluster for each of these values can be seen in Figure 3. From these figures, it can be noted that a higher drift probability results in a denser cluster. This is a logical result since, for a higher probability, the particles move mostly in one same direction and perform less of a random walk (less likely for there to be empty areas inside the cluster).



a) **b)** **c)**

Figure 3. *Particle drift analysis for clusters with $N = 2500$ particles and* ***a)*** *$P_{drift} = 0.1$,* ***b)*** *$P_{drift} = 0.5$, and* ***c)*** *$P_{drift} = 1$*

This visual result also agrees with the fractal dimension values calculated, as seen in Figure 4. Increasing the drift probability results in an increase in fractal dimension. Specifically, for a $P_{drift} = 0.1$, 0.5 and 1, $D_f = 1.626 \pm 0.005$, 1.663 ± 0.006 and 1.697 ± 0.005, respectively. The reasoning behind these results is that, for a lower P_{drift}, the particles perform more of a random walk and thus are more likely to stick to the sides of the cluster arms. Therefore, the cluster grows in different directions, leaving more space inside without any particles (hence the larger radius for the same number of particles). On the other hand, a greater P_{drift} , such as 1, ensures that the cluster grows mostly in one direction and this decreases the chance for the cluster to grow sideways, for example. The main challenge encountered with this algorithm was being able to show the difference in density of the structures, since it was difficult to visualize when considering different values of P_{drift}. For this reason, three values were selected with a significant difference between each. It is likely that running the code for a much larger number of particles would make the difference between closer values of P_{drift} more notable.

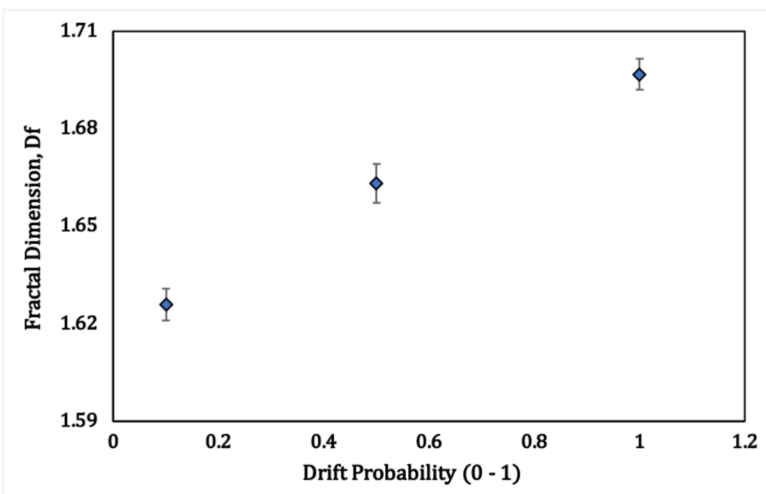


Figure 4. *Fractal dimension values showing an increase with higher drift probability*

iii) <u>Inwards fractal growth and sticking probability analysis</u>

The results from the algorithm that grows fractal structures inwards from a circle with a set radius are shown in Figure 5. The color scheme in this case begins with the red particles as the first ones to be aggregated, followed by the green and yellow, respectively. For a set number of particles (2500), it can be clearly noted that lower sticking probabilities result in really dense structures where the circular domain is not explored as much as for higher probabilities. In fact, for a sticking probability of 1 (assumed for the DLA base case), the system is not even able to reach 2500 particles before reaching the center of the circle in some cases, as shown in Figure 5d. This also occurred rarely for $P_{stick} = 0.5$. A solution to this could have been to increase the initial radius size, however it would have been difficult to visualize the fractal structures at the very low probabilities.

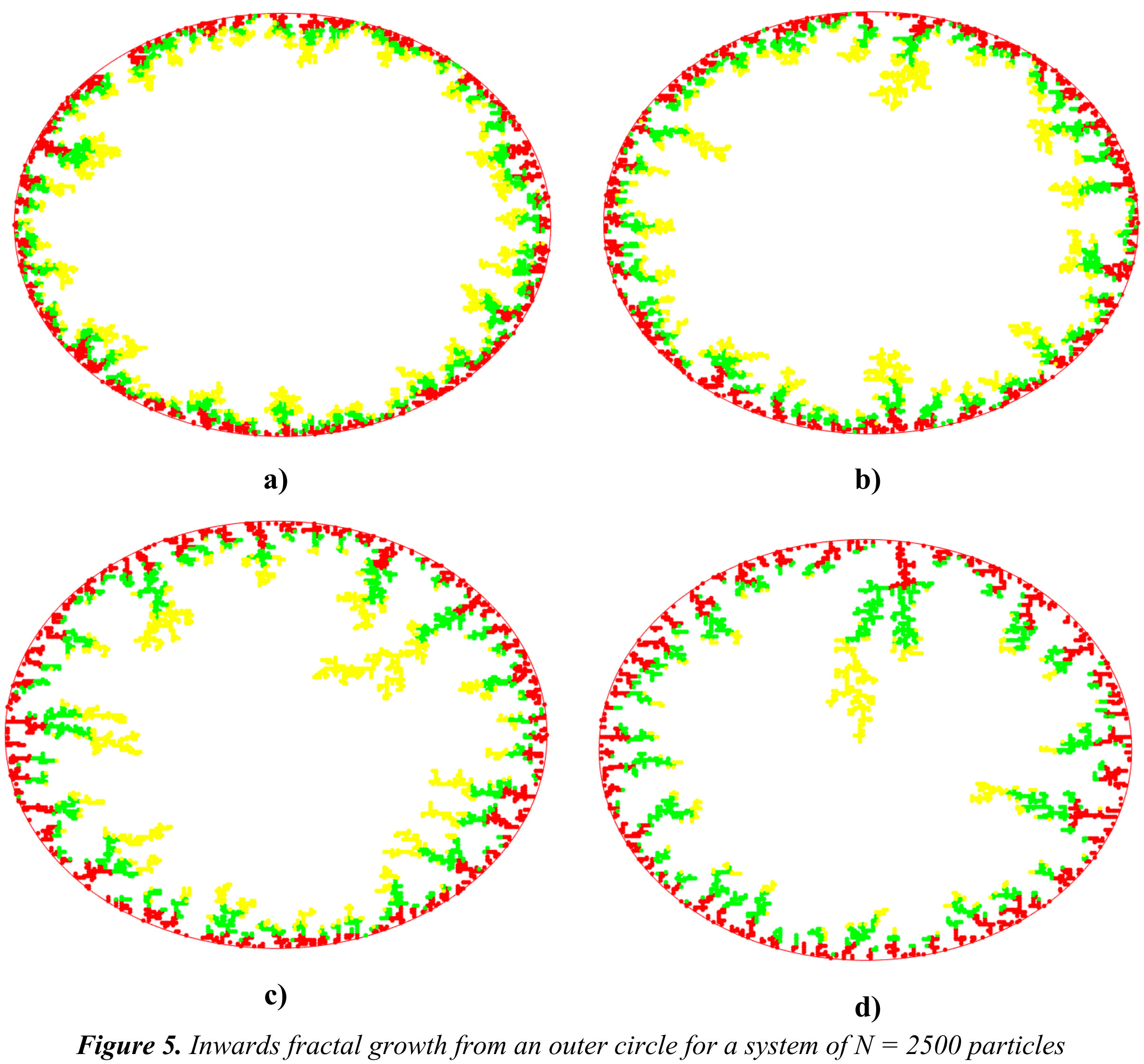


Figure 5. *Inwards fractal growth from an outer circle for a system of $N = 2500$ particles and a) $P_{stick} = 0.1$, b) $P_{stick} = 0.25$, c) $P_{stick} = 0.5$, and d) $P_{stick} = 1$ ($N < 2500$)*

As with the particle drift analysis, the visual representation of these structures agrees with the fractal dimension values calculated, shown in Figure 6. The fractal dimension of the system significantly increases when decreasing the sticking probability, since there are more particles aggregated within a smaller area. Specifically, for a P_{stick} = 1, 0.5, 0.25 and 0.1, D_f = 1.750 ± 0.008, 1.769 ± 0.005, 1.820 ± 0.007 and 1.864 ± 0.005, respectively. In the case of varying this sticking parameter, once again a difficulty was encountered when analyzing values that are close together. Especially for the range of P_{stick} = 0.5 – 1, the change in fractal dimension is not very significant as well as the visual difference of the structures. However, as the value of the parameter continues to decrease, the change in fractal dimension and appearance of the system is more notable.

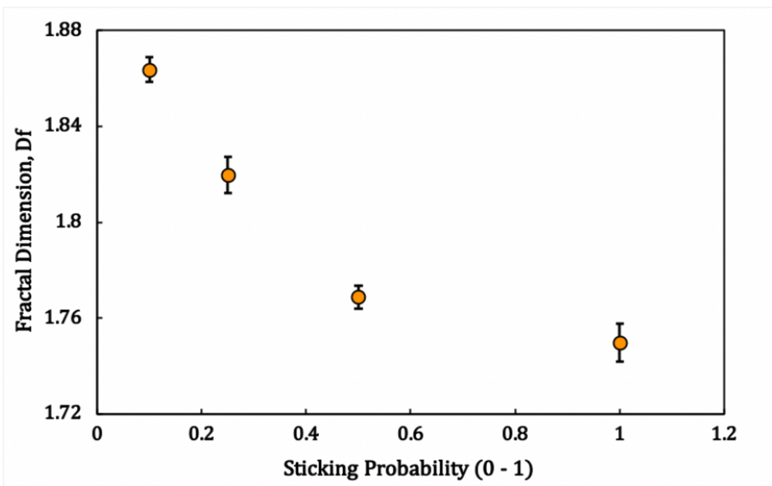


Figure 6. *Fractal dimension values showing an increase with lower sticking probability*

IV. Conclusions

The fractal dimension values obtained for the base case DLA cluster by two different methods agreed with that of previous findings in this field ($D_f \approx 1.71 - 1.77$). It was found that the more direct method of looking at the radius and number of particles for the final cluster, instead of taking many values throughout the run, provided more consistent results with lower error. Therefore, such method was used for the rest of the analyses in the study. In addition, the standard error of all the values calculated was significantly low and, even with the highest deviation from the mean, the values are still within the desired range.

The additional analyses performed by varying different parameters also agreed with expectations based on the concept of diffusion-limited aggregation. When there is a high probability of drift on a particle, the fractal structure that results will be denser and have a higher fractal dimension than when there is no drift and the process is totally random. Additionally, when there is a low probability for each particle to stick to the cluster, it provides more time and space for the particle to explore and thus aggregate in more constrained inner areas of the cluster (greater D_f). A possible limitation of the system that grows fractal structures from a circle and inwards is that more than one structure is being formed (as opposed to one in the base case). Although the trends and general concept of the system are logically correct, it may not be completely accurate to compare specific D_f values of the base case versus the 'creative' case.

V. References

[1] T. Witten and L. Sander, "Diffusion-Limited Aggregation, a Kinetic Critical Phenomenon", Physical Review Letters, vol. 47, no. 19, pp. 1400-1403, 1981. Available: 10.1103/physrevlett.47.1400.

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