

Diffusion-limited aggregation

(PHYS 3142 Final Project[1])

He Zhiwei

Physics Department

Hong Kong University of Science and Technology

Clear Water Bay, Hong Kong

Abstract

In this report, we present a study of the Diffusion-limited aggregation (DLA) process using the Monte Carlo method in Python. Our simulation method is based on the classic algorithm proposed by Witten and Sander, and we extend it to consider various scenarios, including general cases, density function and fractal dimension analysis. Moreover, we investigate the effects of different parameters on the DLA process, such as introducing Psnn, varying probabilities on direction, real boundary, 3D DLA, and different seed configurations. To enhance the visualization of our simulation results, we create animations and produce beautiful DLA images. Our study provides valuable insights into the DLA process and demonstrates the versatility of our simulation method.

Keywords: *Keyword 1; keyword 2; keyword 3; keyword 4; keyword 5*

*He, Zhiwei E-mail address: zhebc@connect.ust.hk

1. Introduction

Diffusion-limited aggregation (DLA) is a mathematical model used to describe the process by which particles undergoing a random walk due to Brownian motion cluster together to form aggregates. The theory was first proposed by Witten and Sander in 1981 and is applicable to aggregation in any system where diffusion is the primary means of transport. DLA is observed in a variety of systems, including electrodeposition, Hele-Shaw flow, mineral deposits, and dielectric breakdown.

DLA has found widespread application in fields such as physics, chemistry, materials science, and computer graphics. It is often used to model the growth of crystals, the formation of snowflakes, and the aggregation of particles in a fluid. In DLA, particles are allowed to move randomly through a medium until they come into contact with other particles, at which point they become "stuck" and begin to form a larger aggregate. The resulting patterns often exhibit fractal-like structures, with self-similar shapes at different scales.

In this report, we will simulate the DLA process in different situations and analyse its density function and fractal dimension, attached with animation and beautiful picture.

2. Methods

A model for simulating diffusion-limited cluster aggregation was proposed by Witten and Sander and later developed by Meakin. The model and algorithm use the Monte Carlo method and a two-dimensional simple cubic lattice, where particles occupy only lattice sites.

Initially, a seed particle is placed at the center and a new particle is added at a sufficiently far distance and undergoes a random walk over the lattice via successive random jumps to one of the four nearest neighbor sites. The probability of a jump to any of the nearest neighbor sites is the same and normalized to have an overall jump probability equal to unity. Once the moving particle reaches one of the sites adjacent to the seed, it could be attached to the seed according to the sticking probability at the nearest neighbor sites (P_{nn}) and the sticking probability at the second nearest neighbor sites (P_{snn}). For simplicity, we consider only the nearest neighbor interaction (setting $P_{nn} = 1$ and $P_{snn} = 0$). During the simulation, each of the first nearest neighbor sites is checked after each jump, and if the particle sticks to the cluster at one of the nearest neighboring sites, the checking is stopped. This approach is equivalent to computing the conditional probabilities for the moving particle to stick at each of the nearest sites but works faster if implemented in the simulation. If the particle doesn't stick to the nearest neighbor sites for the first time, it continues the random walk until it attaches to the cluster or moves too far from it. In the latter case, the particle is deleted from the lattice and starts over again from a distance closer to the cluster. After the first particle attaches to the cluster, a second particle is introduced and undergoes the same procedure to form the cluster. The particles are started at a distance $R_{max} + 5$ from the cluster, where R_{max} is the maximum distance from the seed to the outermost particle in the cluster, and all distances are measured in units of the lattice spacing. If the

particle moves further than $3R_{max}$ from the cluster, it is killed and started again at a random position on the circle of radius $R_{max} + 5$ centered at the same point as the seed particle. To decrease computational time, the checking of the nearest neighbor sites is started only if the particle reaches the distance $R_{max} + 2$ from the cluster. A schematic depiction of the system is shown in the following figure 1. Different values for the radius of the start-off circle and the distance at which the particle is killed were used, and the corresponding results were the same within a statistical error.

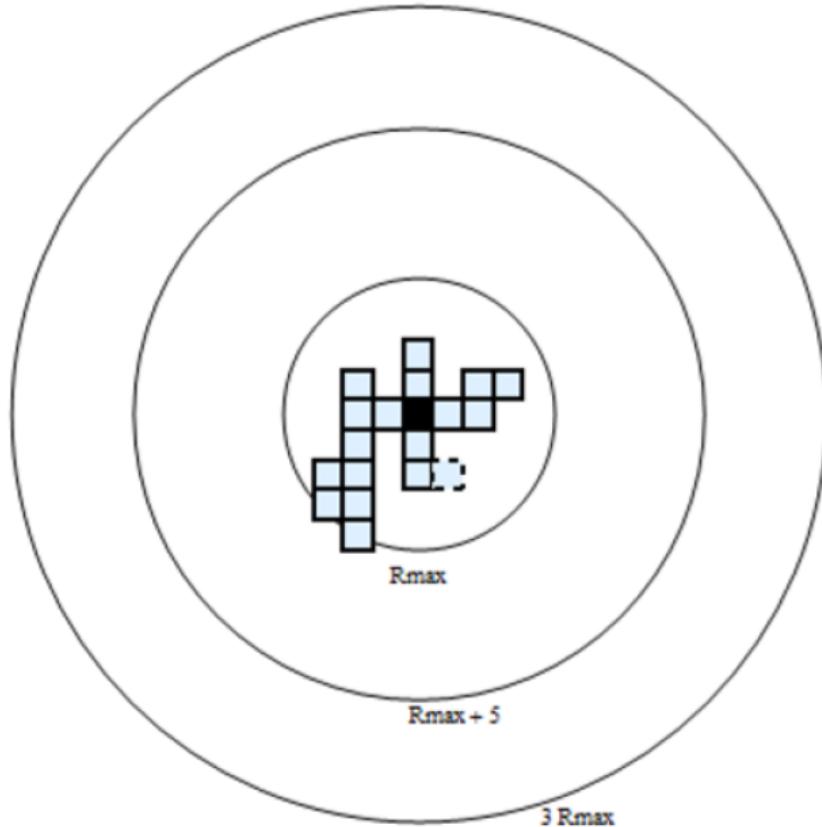


Figure 1

3. Result and Discussion

3.1. (a)General case($P_{nn} = 1$)

In this part, we use the typical two-dimensional cluster model and the algorithm above to grow $N=10000$ particles and plot the figure where the seed particle fixed at the center of the figure.

The nearest sticking probability (P_{nn}) is set to 1, and the size of the lattice is 500. We plot the figure 2:

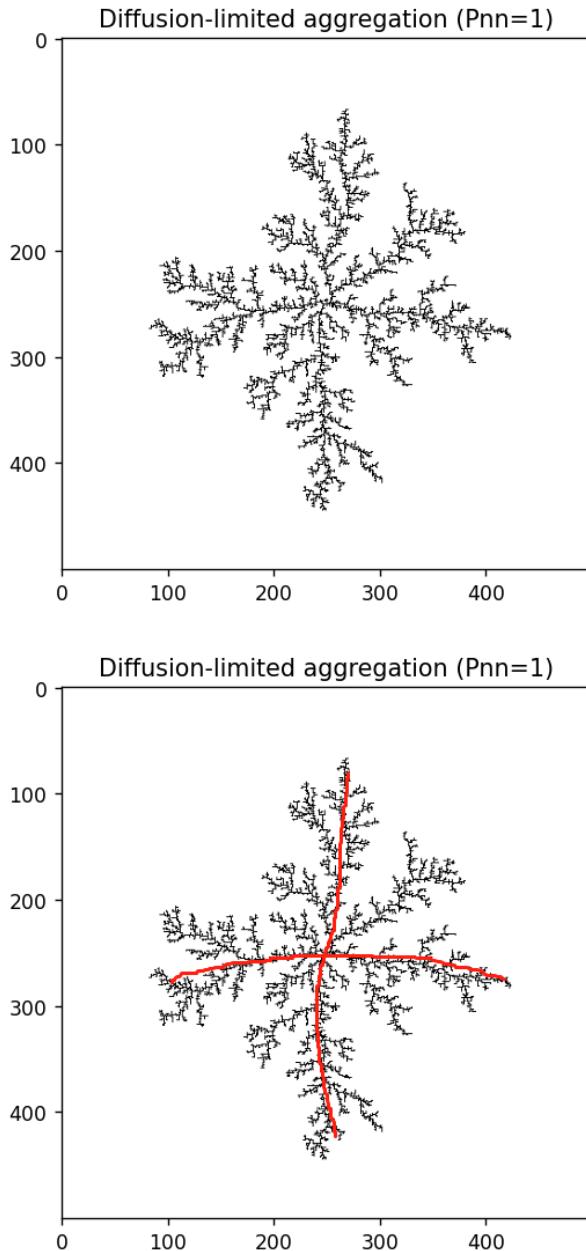


Figure 2. **Top.** DLA simulation with grid size=500, N=10000, and $P_{nn} = 1$.
Bottom. DLA simulation pattern presents a central corss structure

As the particles are only able to random walk and adhere to the existing cluster in four directions (up, down, left, and right), the resulting growth pattern exhibits a distinct central cross structure, as indicated by the red line in the bottom of Figure 2.

3.2. (b)General case($P_{nn} = 0.3$)

In Part (b), we repeat the simulation using the same lattice model and algorithm to grow N=10000 particles, but with a reduced P_{nn} of 0.3. The resulting figure,

shown in Figure 3, illustrates the impact of a lower sticking probability on the growth pattern.

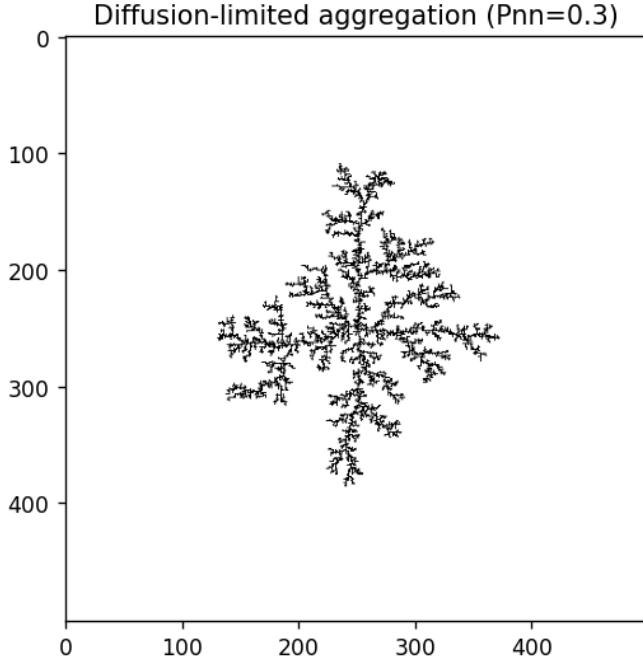


Figure 3. DLA simulation with grid size=500, N=10000, and $P_{nn} = 0.3$

Specifically, particles approaching the cluster have a reduced likelihood of adhering at the first instance due to the decreased P_{nn} . Consequently, the detachment of the cluster is increased, leading to a higher likelihood of particle aggregation closer to the center. As a result, the pattern of aggregation appears denser compared to the $P_{nn}=1$ case.

3.3. (c)Density function and (d)Fractal dimension

In order to further analyze the growth patterns observed in the previous section, we define a density function $C(r)$, which represents the number of particles located at a distance r from the reference particle for all particles in the cluster. This density function is then normalized using the total number of particles and the corresponding volume between two spheres of radius $(r - \delta r)$ and $(r + \delta r)$, respectively.

To determine the relationship between $\ln(C(r))$ and r for both $P_{nn}=1$ and $P_{nn}=0.3$, we calculate the density function exponent α using the power law dependency $C(r) \sim r^{-\alpha}$. The fractal dimension D can then be obtained using the relationship $D = d - \alpha$, where d is the Euclidean dimension.

To calculate α , we first determine the number of particles within different r values, denoted as $N(r)$. We assume that $N(r) = Nr^a$ and $C(r) = Cr^{-\alpha}$, and then take the logarithm of both sides to obtain

$$\ln(N(r)) = a\ln(r) + \ln N$$

and

$$\ln(C(r)) = (-\alpha)\ln(r) + \ln C$$

The relationship between $N(r)$ and $C(r)$ can be written as

$$N(r) = \int (C(r) \times 2\pi r) dr$$

allowing us to solve for the parameter relationship

$$-\alpha = a - 2$$

and

$$\ln C = \ln\left(\frac{a}{2\pi}\right) + \ln N$$

Using a valid range of r values, we fit the logarithm of $N(r)$ and then obtain $\ln(C(r))$. The resulting plots for $P_{nn}=1$ and $P_{nn}=0.3$ are shown in Figures 4 and 5, respectively. In addition, the fractal dimension $D = d - \alpha$ is just 'a' we calculated before.

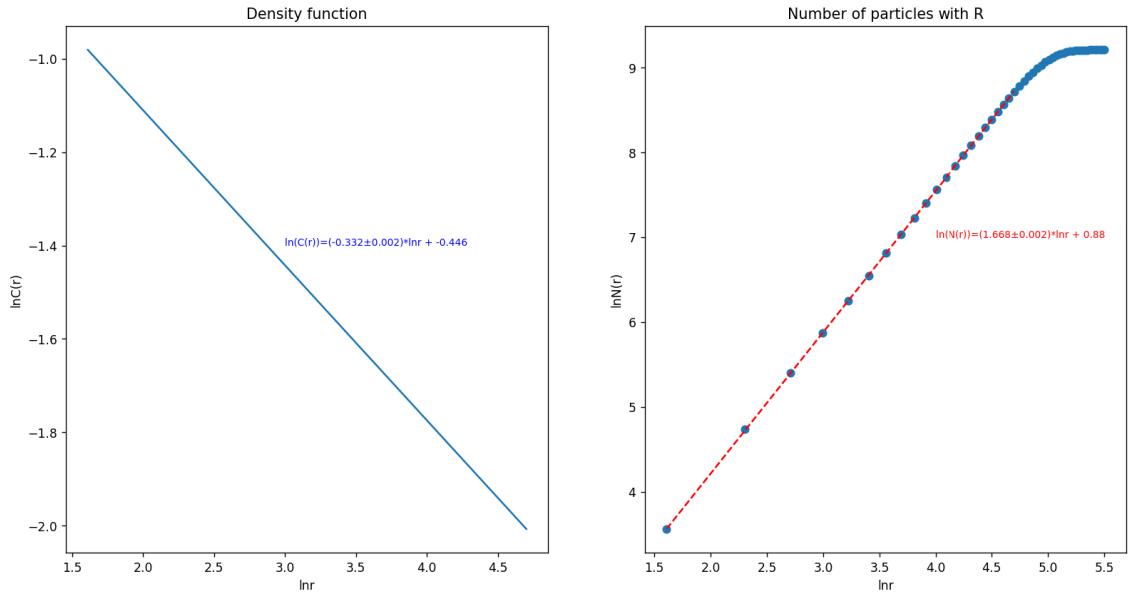


Figure 4. Size of lattice 500, $N=10000$, $P_{nn}=1$ and simulation 20 clusters: Left shows the **Density function** $C(r)$. Right shows **Number of particles with N**(blue points) and linear fit function of $N(r)$ (red line)

The result shows that the $\alpha = 0.332 \pm 0.002$ which is agree with [2] within acceptable error, and the fractal dimension D is 1.668 ± 0.002 .

$$\ln(C(r)) = (-0.332 \pm 0.002) \ln r - 0.446$$

$$\ln(N(r)) = (1.668 \pm 0.002) \ln r + 0.88$$

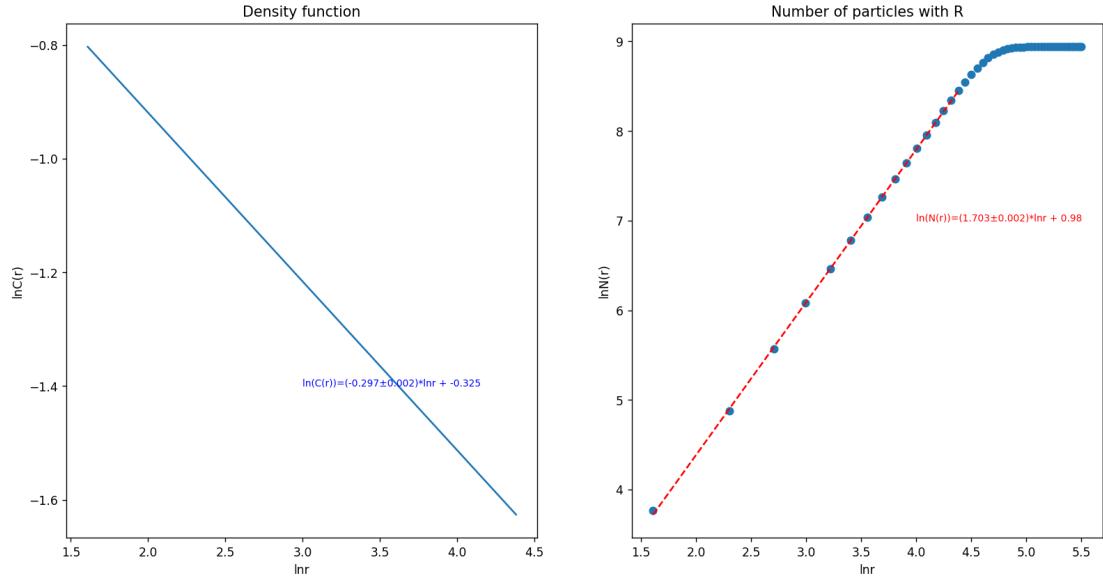


Figure 5. Size of lattice 500, $N=10000$, $P_{nn}=0.3$ and simulation 20 clusters: Left shows the **Density function** $C(r)$. Right shows **Number of particles with R**(blue points) and linear fit function of $N(r)$ (red line)

The result shows that the $\alpha = 0.297 \pm 0.002$ and the fractal dimension D is $1.703 \pm 0.002 > 1.668$. It means that $P_{nn}=0.3$ is denser than $P_{nn}=1$, which agrees with the analysis above.

4. (e)Further discussion

4.1. ①Introduce P_{snn}

Then we consider $P_{snn} = \frac{1}{2}P_{nn}$ while $P_{nn}=1$ or 0.3.

Plot the figure for $P_{nn} = 1$, $P_{snn} = 0.5$ below:

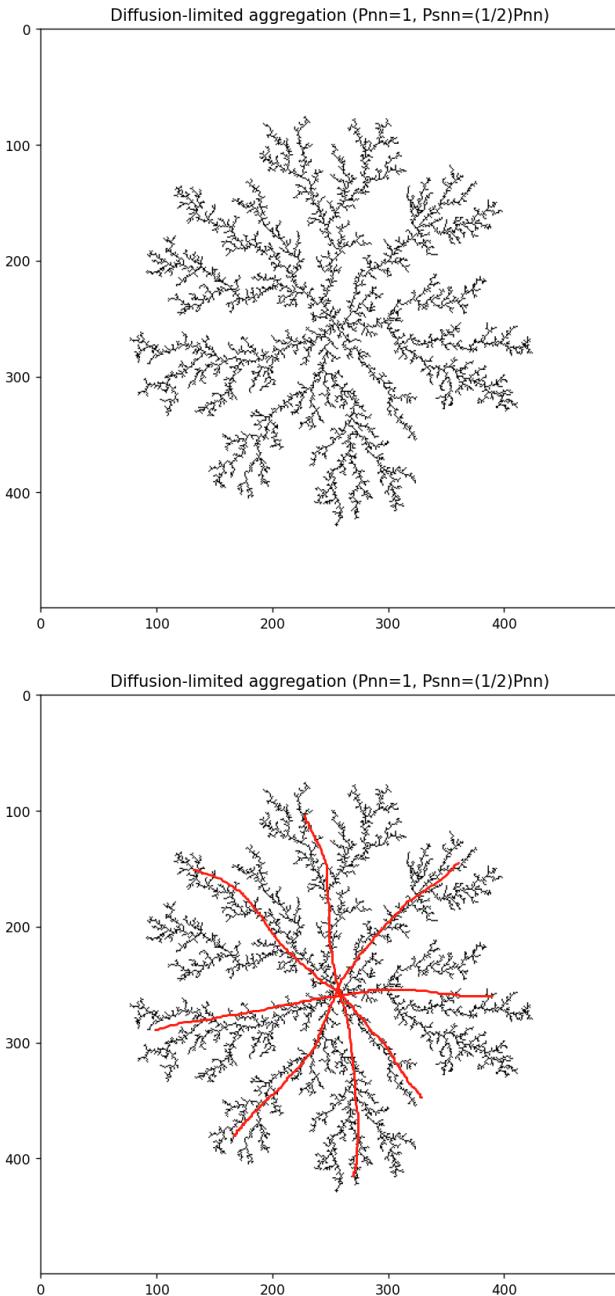


Figure 6. Top. DLA simulation with grid size=500, N=10000, and $P_{nn} = 1, P_{snn} = 0.5$. **Bottom.** DLA simulation pattern presents a central double cross structure

Given that particles can stick to the cluster in eight directions, the resulting growth pattern exhibits a distinct central double cross structure, as indicated by the red line in the bottom of Figure 8. Moreover, due to the increased number of possible sticking directions, the growth pattern is expected to be denser compared to the cases of $P_{nn} = 1, P_{snn} = 0$.

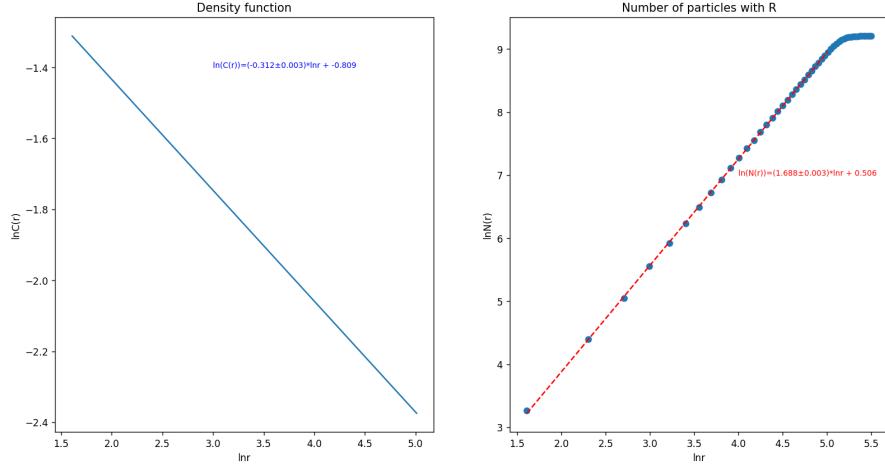


Figure 7. Size of lattice 500, $N=10000$, $P_{nn} = 1$, $P_{snn} = 0.5$ and simulation 10 clusters: Left shows the **Density function** $C(r)$. Right shows **Number of particles with N**(blue points) and linear fit function of $N(r)$ (red line)

The result shows that the $\alpha = 0.312 \pm 0.003$ and the fractal dimension D is $1.688 \pm 0.003 > 1.668$. It means that $P_{nn} = 1$, $P_{snn} = 0.5$ is denser than $P_{nn} = 1$, $P_{snn} = 0$, which is as expected.

Plot the figure for $P_{nn} = 0.3$, $P_{snn} = 0.15$ below:

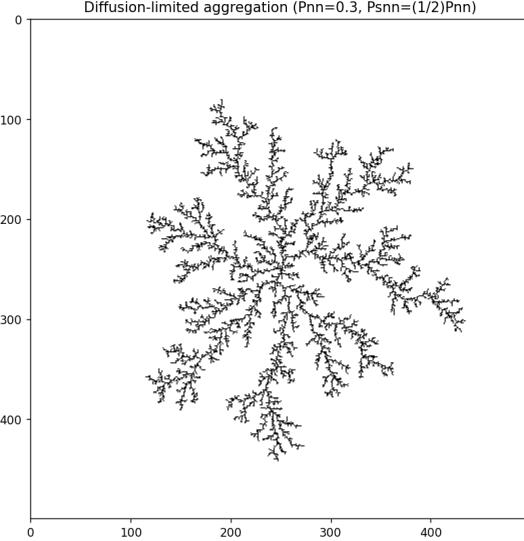


Figure 8. DLA simulation with grid size=500, $N=10000$, and $P_{nn} = 0.3$, $P_{snn} = 0.15$.

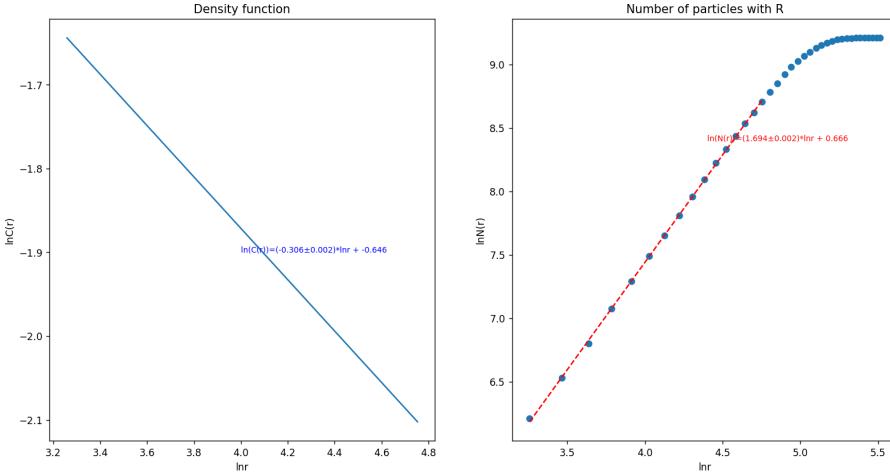


Figure 9. Size of lattice 500, $N=10000$, $P_{nn} = 0.3$, $P_{snn} = 0.15$ and simulation 5 clusters: Left shows the **Density function** $C(r)$. Right shows **Number of particles with N** (blue points) and linear fit function of $N(r)$ (red line)

The result shows that the $\alpha = 0.309 \pm 0.002$ and the fractal dimension D is 1.694 ± 0.002 . It is denser than $P_{nn} = 1$, $P_{snn} = 0.5$ by the same reason as general case, which is as expected.

4.2. ②Different probabilities on direction

We can explore the effect of directional bias on the growth pattern of DLA by introducing probabilities that differ for different directions during the random walk of a particle.

Example A: $P_{left}=0.1$, $P_{right}=P_{up}=P_{down}=0.3$, $N=10000$,

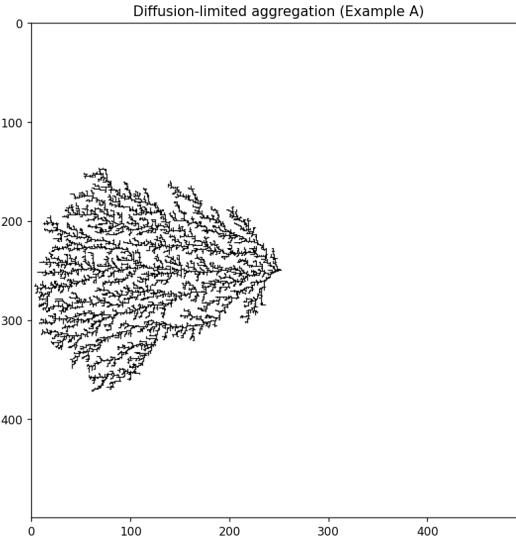


Figure 10. DLA simulation with grid size=500, $N=10000$, and $P_{left}=0.1$, $P_{right}=P_{up}=P_{down}=0.3$.

Due to the higher probability of sticking from the right side of a particle compared to the left side, particles tend to aggregate on the left side of the cluster. As a result, the overall pattern of aggregation exhibits a bias towards the left, as illustrated in Figure 10.

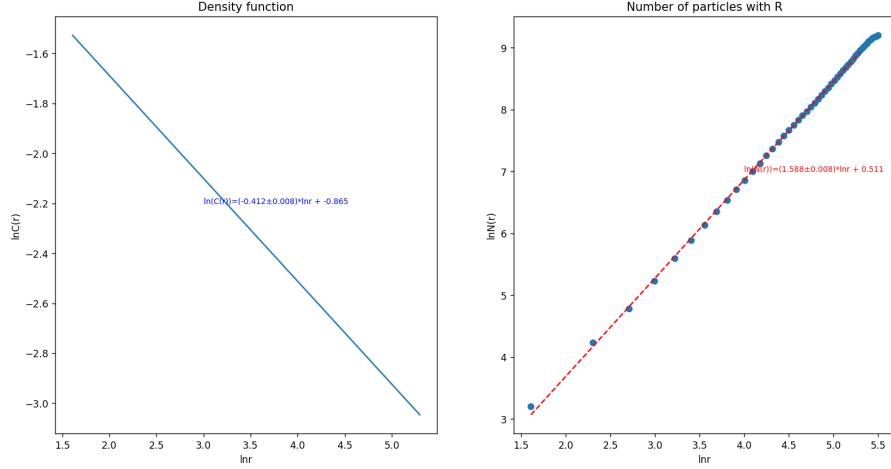


Figure 11. Size of lattice 500, $N=10000$, $P_{left}=0.1$, $P_{right}=P_{up}=P_{down}=0.3$, and simulation 5 clusters: Left shows the **Density function** $C(r)$. Right shows **Number of particles with N**(blue points) and linear fit function of $N(r)$ (red line)

The result 11 shows that the $\alpha = 0.412 \pm 0.008$ and the fractal dimension D is 1.588 ± 0.008 . This means that it is sparse.

Example B: $P_{left}=P_{right}=0.1$, $P_{up}=P_{down}=0.4$, $N=5000$,

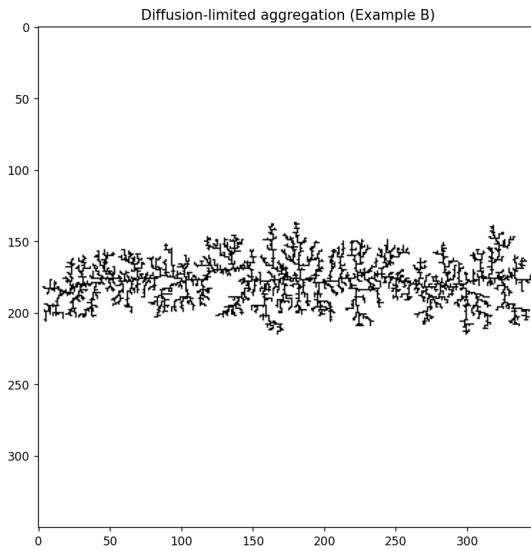


Figure 12. DLA simulation with grid size=350, $N=5000$, and $P_{left}=P_{right}=0.1$, $P_{up}=P_{down}=0.4$.

Since there is a higher probability of sticking from the top and bottom sides of a

particle compared to the left and right sides, particles tend to aggregate on the left and right sides of the cluster. As a result, the overall pattern of aggregation exhibits a bias towards the left and right sides, as illustrated in Figure 12.

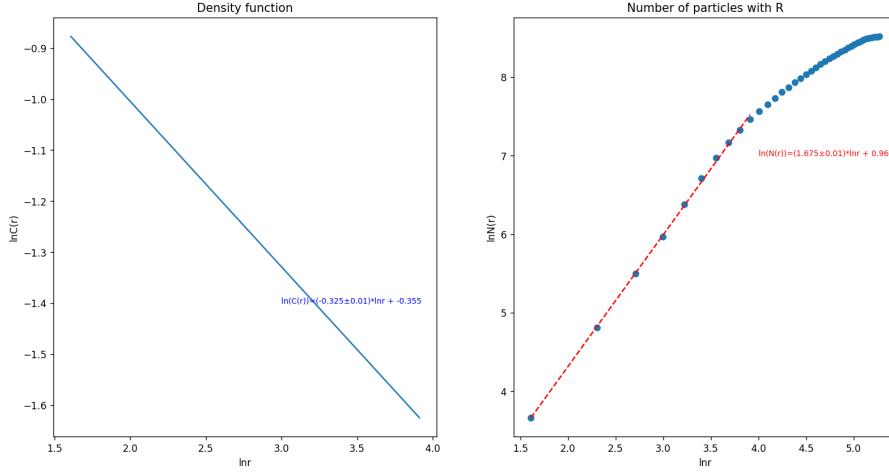


Figure 13. Size of lattice 400, $N=5000$, $P_{left}=P_{right}=0.1$, $P_{up}=P_{down}=0.4$, and simulation 5 clusters: Left shows the **Density function** $C(r)$. Right shows **Number of particles with N**(blue points) and linear fit function of $N(r)$ (red line)

The result shows that the $\alpha = 0.32 \pm 0.01$ and the fractal dimension D is 1.67 ± 0.01 . The observation of a potential division in the density function at $R = 55$ may indicate a change in the growth pattern or the presence of a boundary effect.

4.3. (3)Real boundary

In order to introduce a realistic boundary, we set a parameter R_b that limits the maximum distance a particle can travel during a random walk. Specifically, particles are not "killed" or removed from the simulation when they move further than 3 times the maximum radius of the cluster (R_{max}). Instead, they are allowed to continue their random walk until they reach a distance of R_b , at which point they stop and proceed to the next random walk. If the particle encounters the cluster during this random walk, it will adhere to the existing cluster.

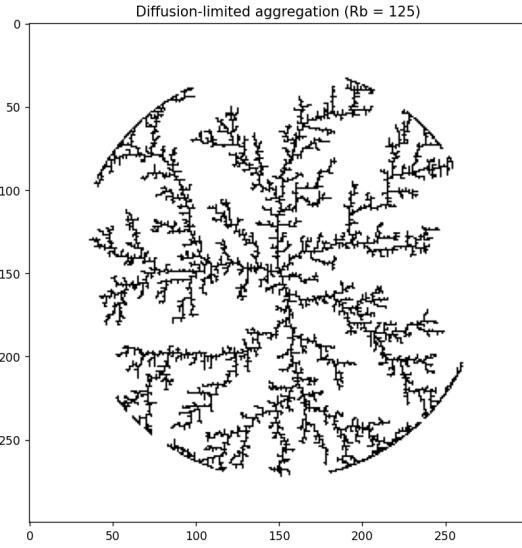


Figure 14. DLA simulation with lattice size=300, N=9000, and Rb=125.

To demonstrate the effect of real boundaries, we reduce the size of the lattice and introduce the parameter R_b as previously described. Due to this boundary condition, particles are limited by a circle with radius R_b , as illustrated in the accompanying figure 14.

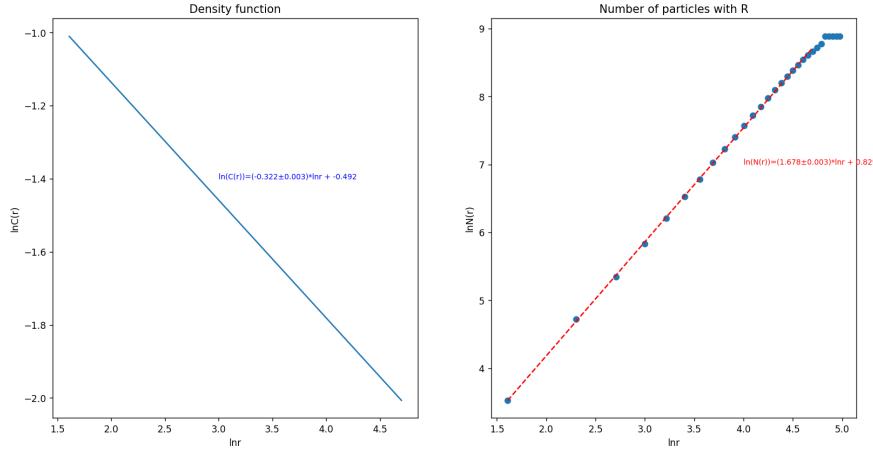


Figure 15. Size of lattice 300, N=9000, Rb=125, and simulation 7 clusters: Left shows the **Density function** $C(r)$. Right shows **Number of particles with R** (blue points) and linear fit function of $N(r)$ (red line)

The resulting analysis with the introduced boundary condition indicates a density function exponent of $\alpha = 0.322 \pm 0.003$ and a fractal dimension D of 1.678 ± 0.003 . Due to the presence of the boundary limiting particle diffusion, the resulting growth pattern is slightly denser than the general case without a boundary. However, the overall growth pattern remains similar.

4.4. ④Three-dimensional DLA

We then extend the simulation to three-dimensional DLA. In order to avoid long computation time, we reduce the lattice size to 150 ($150 \times 150 \times 150$) and simulate the growth of $N=5000$ particles in each run. To visualize the resulting growth pattern, we color the figure based on the time at which particles aggregate, as illustrated below.

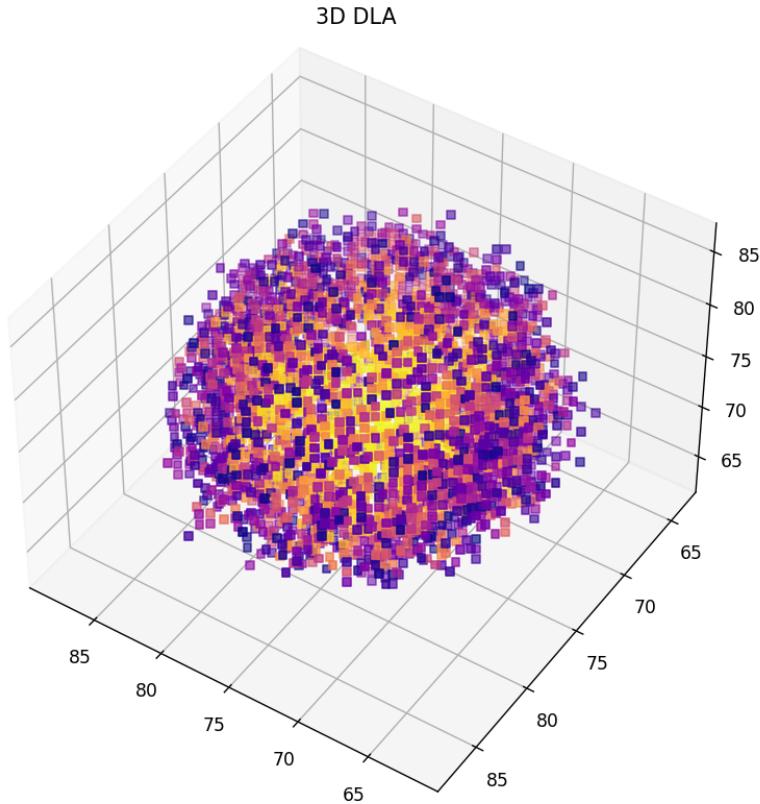


Figure 16. DLA simulation with lattice size=150, $N=5000$.

We observe that the growth pattern of the plane projection of the three-dimensional Diffusion Limited Aggregation is similar to the 2D general case, which is as expected.

To analyze the density function and fractal dimension of the 3D DLA, we need to modify the equations used in the 2D case. Specifically, the relationship between N and C can be written as:

$$N(r) = \int (C(r) \times 4\pi r^2) dr$$

Thus, the parameter relationship is modified to:

$$-\alpha = a - 3$$

$$\ln C = \ln\left(\frac{a}{4\pi}\right) + \ln N$$

These modifications allow us to calculate the density function exponent α and the fractal dimension D , which represents the degree of branching and complexity of the 3D DLA structure.

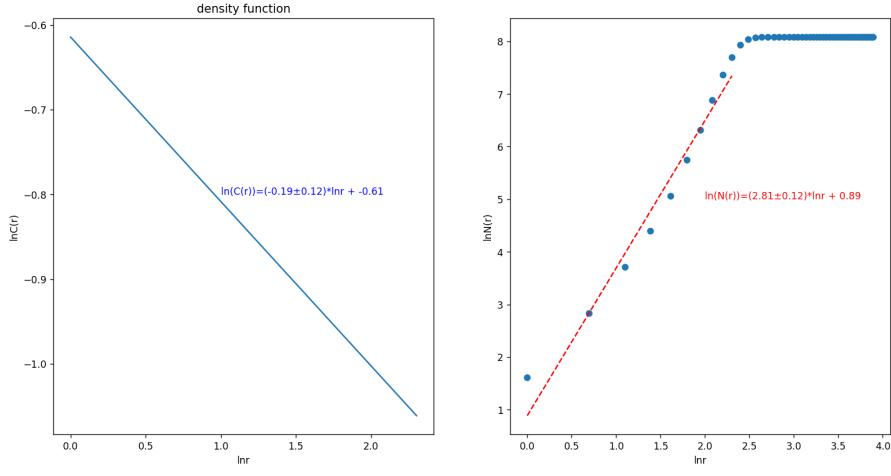


Figure 17. Size of lattice 150, $N=5000$, and simulation 10 clusters: Left shows the **Density function** $C(r)$. Right shows **Number of particles with N** (blue points) and linear fit function of $N(r)$ (red line)

Analysis of the density function and fractal dimension of the 3D DLA yields a density function exponent of $\alpha = 0.19 \pm 0.12$ and a fractal dimension D of 2.81 ± 0.12 . These results indicate a highly complex and branched structure, with a much higher degree of branching and complexity compared to the 2D DLA case. The relatively large error bars in the measured values reflect the inherent variability and randomness inherent in the DLA simulation.

4.5. ⑤Different Seeds

We can also investigate how the growth pattern is influenced by the initial seed configuration. In particular, we can consider different types of seed arrangements, such as multiple seeds, seeds with line or circle shape, and seeds placed along the border of the lattice. By examining the growth pattern resulting from different seed configurations, we can gain insights into the role of initial conditions in shaping the final structure of the DLA.

4.5.1. Multiple seeds

Due to the lack of circular symmetry in the non-circular seed configurations, it is not possible to calculate the density function and fractal dimension of the resulting DLA structures. Therefore, we need to adopt a different approach for analyzing these structures.

One possible method is to randomly select a radius R from the two different centers of the seed configuration and use this to generate new particles during the simulation. To aid in visualization, we can color the resulting DLA structure according to the order in which particles were added.

For the case of seeds arranged along the diagonal of the lattice grid, we can randomly select a radius $randR$ from the two diagonal centers to generate new particles during the simulation:

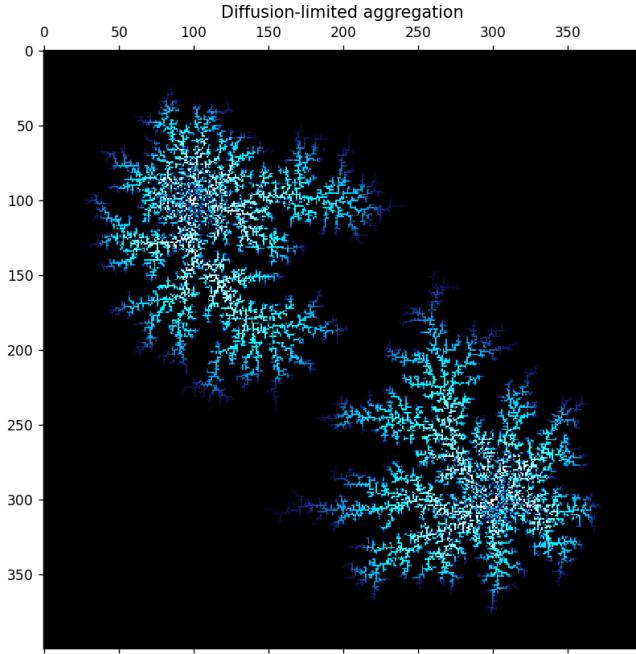


Figure 18. DLA simulation with lattice size=400, N=25000, and 2 seeds.

For the case of seeds arranged both along the diagonal and off-diagonal of the lattice grid, we can randomly select a radius R from the four different centers to generate new particles during the simulation.

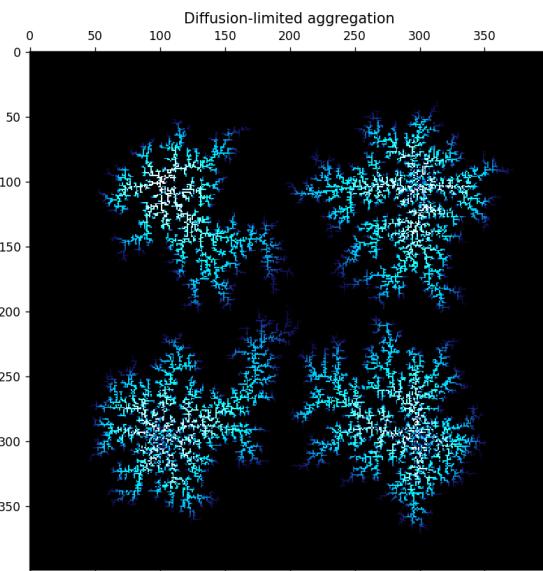


Figure 19. DLA simulation with lattice size=400, N=25000, and 4 seeds.

4.5.2. Line seeds

In the case of line seeds arranged in the lattice grid, the resulting growth pattern lacks circular symmetry, making it impossible to calculate the density function and fractal dimension of the structure.

During the simulation, our initialization method can lead to the growth of the cluster in the middle being restrained by the particles on either side of the line seed configuration. This can result in the formation of an elongated structure with a narrow width, with particles aggregating primarily along the length of the line seed(see fig. 20).

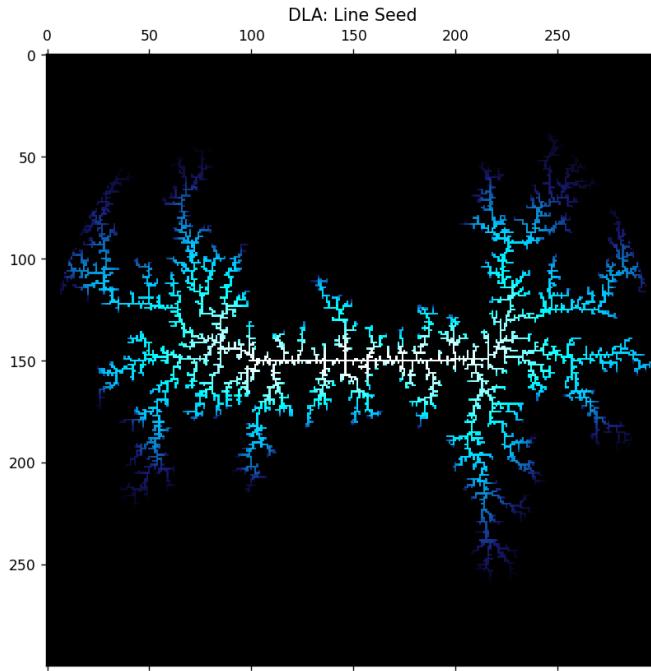


Figure 20. DLA simulation with lattice size=300, N=7000, and linewidth=100.

If we revise the method of updating R_{max} to the farthest vertical distance from the seed, we may be able to relieve the growth restraint resulting from the particle accumulation on either side of the line seed configuration. By updating R_{max} based on the maximum distance from the seed in any direction, rather than just the vertical direction, we can allow the cluster to grow more freely and avoid being constrained by the particles on either side of the line seed(see fig. 21).

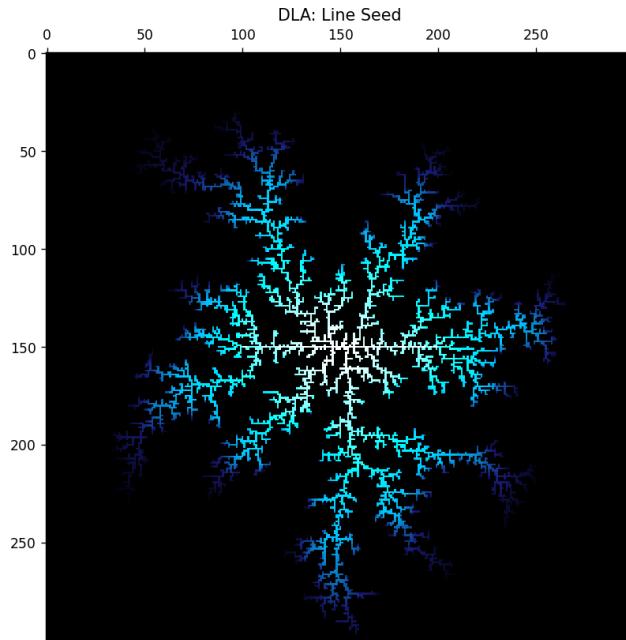


Figure 21. DLA simulation with lattice size=300, N=7000, and linewidth=100.

This comparison shows that the method of generating a random particle is important.

4.5.3. Circular seeds

For the case of circular seeds arranged in the center of the lattice grid, we can analyze the density function exponent and fractal dimension of the resulting DLA structure from the position at radius of the seeds.

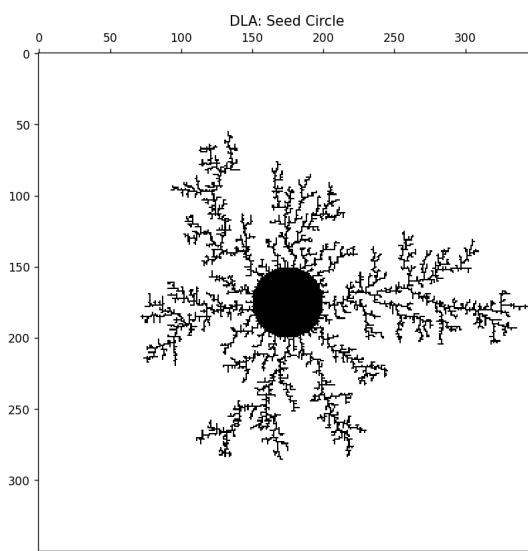


Figure 22. DLA simulation with lattice size=350, N=6000, radius=25.

Its density function and fractal dimension are exhibited:

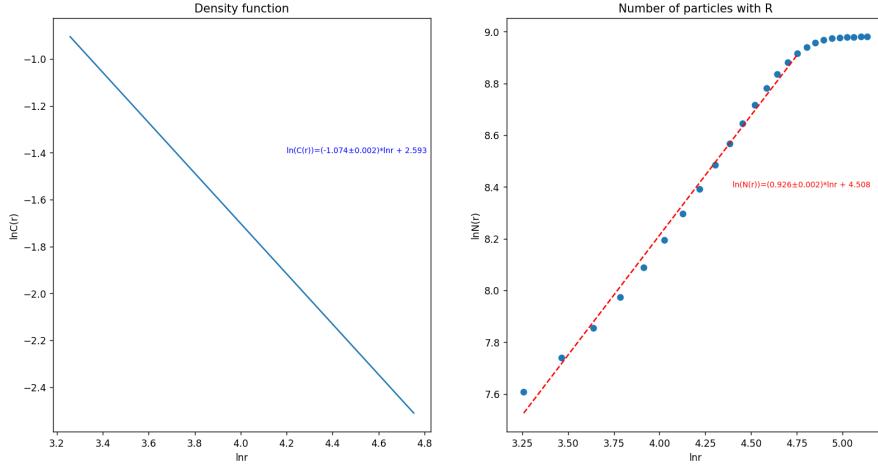


Figure 23. Size of lattice 350, $N=6000$, radius=25, and simulation 5 clusters: Left shows the **Density function** $C(r)$. Right shows **Number of particles with N** (blue points) and linear fit function of $N(r)$ (red line)

The result shows that the $\alpha = 1.074 \pm 0.002$ and the fractal dimension D is 0.926 ± 0.002 . It is very sparse.

4.5.4. border seeds

For the case of seeds arranged along the border of the lattice grid, the resulting growth pattern lacks circular symmetry, making it impossible to calculate the density function and fractal dimension of the structure.

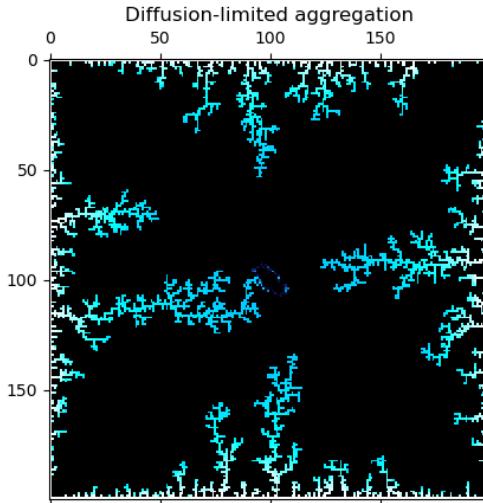


Figure 24. DLA simulation with lattice size=200, $N=10000$, $P_{nn}=0.1$.

However, the resulting growth pattern can still be visually striking and aes-

thetically pleasing, and can provide insights into the complex and highly branched structures

5. Animation Simulation(Recommend to use Adobe DC to open)

In this study, we produced an animation to visualize the growth of the DLA structure. Due to the large amount of data generated during the simulation, it is impractical to use the "matplotlib.animation" module to create the animation directly. Instead, we have saved images at intervals of 100 particles and compiled them into a gif file, and more gifs can be found in the attached files.

Using a lattice size of 400, $N=10000$, and $P_{nn}=1$, we have generated an animation that depicts the growth of the DLA structure. The resulting image appears as if a window is undergoing the freezing process, with particles aggregating in a dense and highly branched pattern.

Using a lattice size of 100, $N=2000$, we have generated an animation that depicts the growth of the 3D DLA structure.

The animation provides a unique visual representation of the DLA process. Further studies employing this method can help to explain the formation of natural structures with complex geometries.

6. Beautiful DLA picture

Here are some colorful and beautiful DLA pictures generated using different parameters and seed configurations:

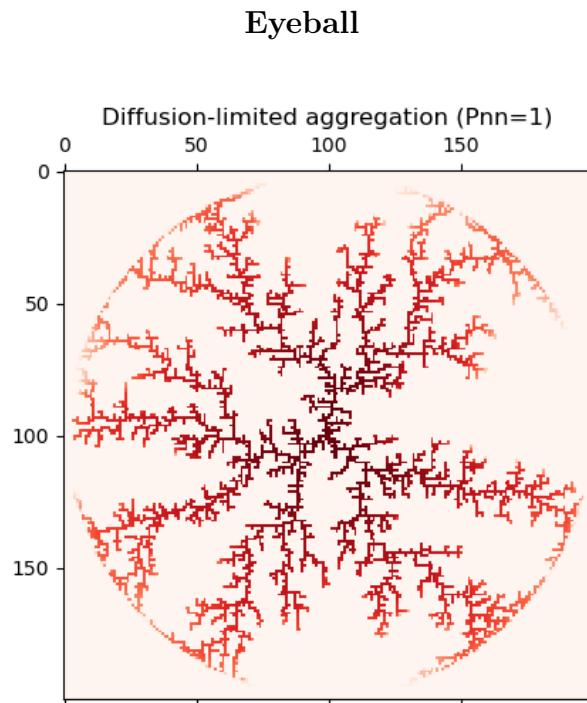


Figure 25. DLA simulation with lattice size=200, N=5000, Rb=100, and camp = 'Reds'.

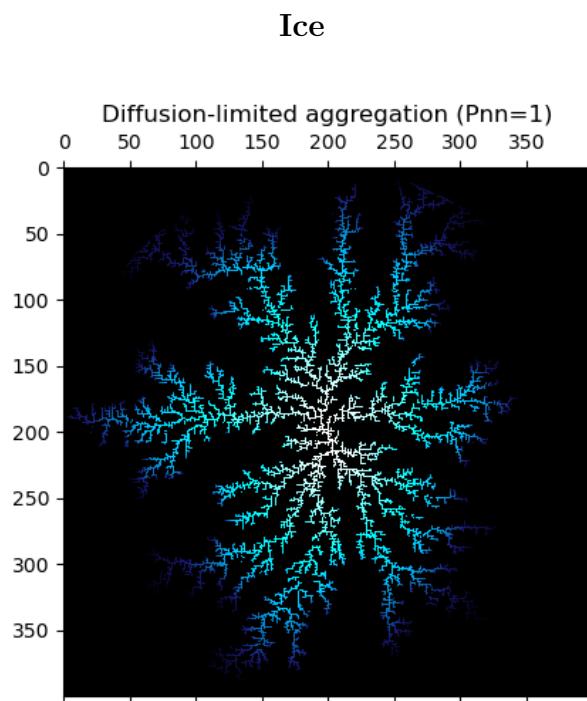


Figure 26. DLA simulation with lattice size=400, N=10000, Pnn=1.

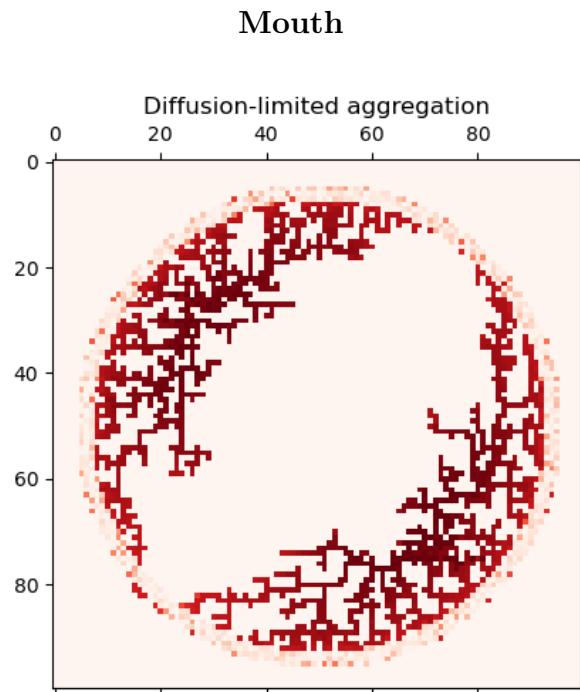


Figure 27. DLA simulation with lattice size=100, N=2000, and 2 seeds.

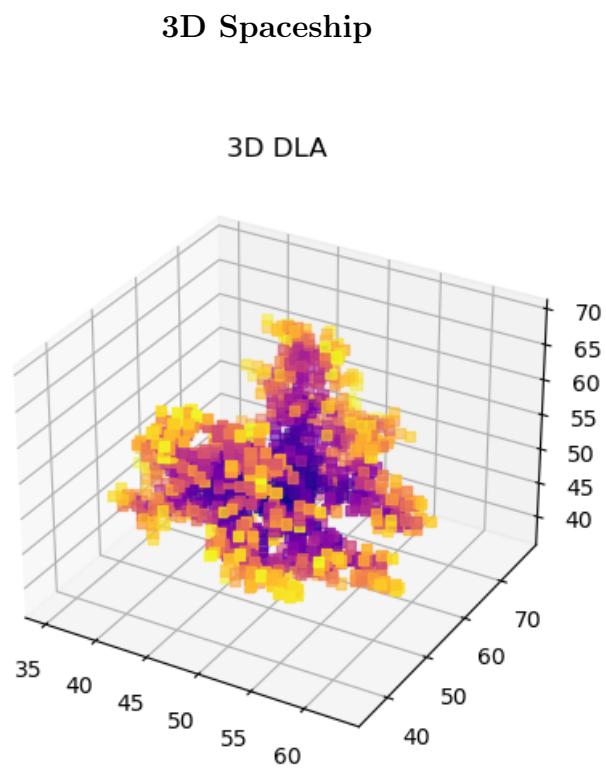


Figure 28. DLA simulation with lattice size=100, N=2000.

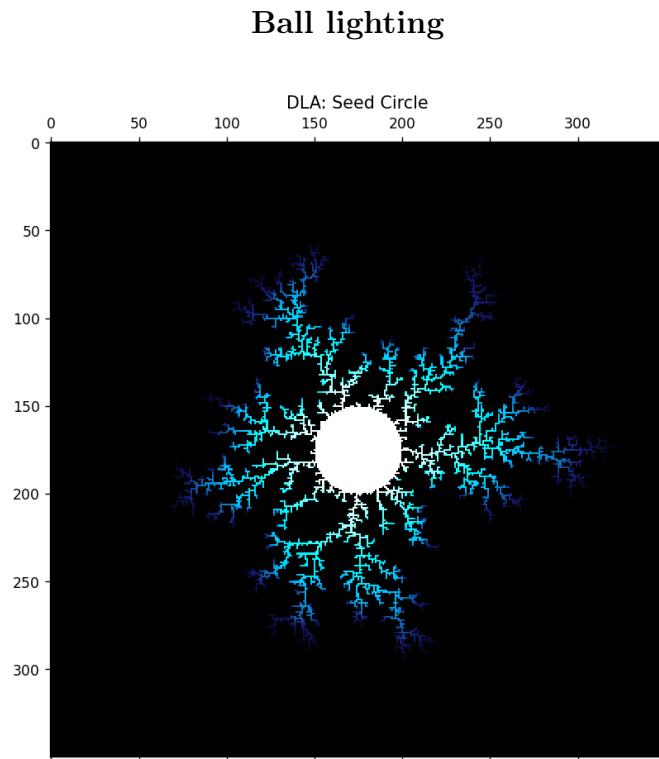


Figure 29. DLA simulation with lattice size=350, N=6000, radius=25.

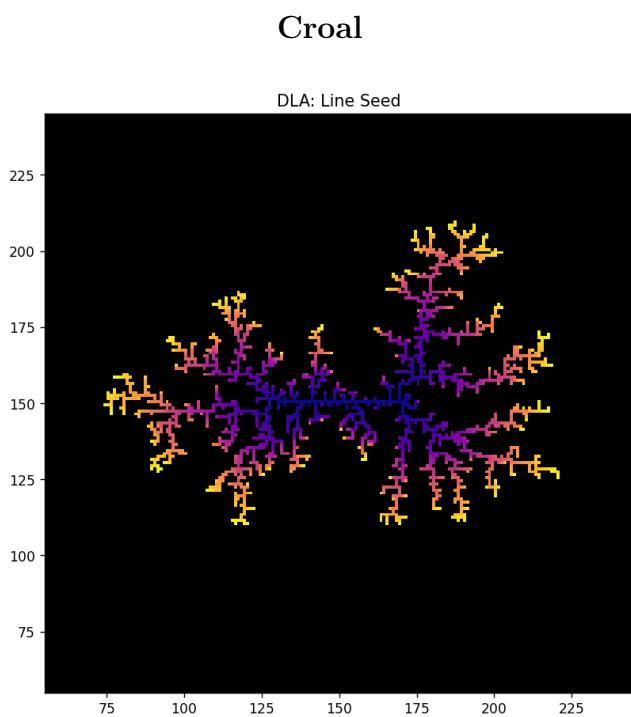


Figure 30. DLA simulation with lattice size=300, N=2000, and linewidth=40.

7. Conclusion

In this report, we have presented a comprehensive study of Diffusion-limited aggregation (DLA), including general cases, density function and fractal dimension analysis, and the effects of different parameters on the DLA process.

Additionally, we have investigated the impact of directional bias, real boundary, 3D DLA, and different seed configurations on the resulting growth pattern. Our study has provided valuable insights into the underlying mechanisms of DLA and demonstrated the versatility of our simulation method.

To enhance the visualization of our simulation results, we have created animations and produced beautiful DLA images. Overall, our study has deepened our understanding of the complex and highly branched structures that can arise from simple diffusion-limited aggregation processes and has demonstrated the importance of considering different seed configurations and parameter values in understanding the resulting growth pattern.

References

- [1] Junwei Liu. Phys 3142 final project. 2023.
- [2] T. A. Witten and L. M. Sander. Diffusion-limited aggregation, a kinetic critical phenomenon. *Phys. Rev. Lett.*, 47:1400–1403, Nov 1981.