Computational simulation of diffusion limited aggregation

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Diffusion limited aggregation (DLA), a common natural growth process, will be simulated, with measurements being made on two simulations. From the radial size of grown clusters, both simulations have the same fractal dimension. Box counting is then used to determine the fractal dimension of a DLA process to 1.716 ± 0.007, a value consistent with numerous published values. To further analyse the process, the simulation is then modified so that not all particles will aggregate onto the cluster after their first collision. Another modification allows for simultaneous simulation of walker particles. Both of these modifications cause the fractal dimension to tend towards a two dimensional object. An equation was found which, in the latter case of simultaneous particles, described the limit for diffusion to dominate the growth of the cluster.

This report is for PH30056 Computational Physics B: Coursework 1.

Code, figures, data and additional appendices can be accessed at `https://edwardwebster.me/dla/`.

I. INTRODUCTION

Diffusion limited aggregation (DLA) is a process where particles (walkers) diffuse through space, sticking together when they come into contact[1], forming a cluster. The cluster formed by DLA processes are fractals, commonly seen in natural growth systems[2]. DLA was first simulated by Witten and Sander[3] who measured the fractal dimension of a small cluster using a computer. Since then major advances in computing technology have allowed for much larger and more complex simulations to be created.

In their paper, Witten and Sander outlined a method for simulating DLA as follows[3]. Simulations create individual walkers which undergo random motion. A cluster is initially created with one seed particle. When the walker encounters a clustered particle, it joins the cluster and can no longer move. A new walker is generated and this too undergoes random motion until it encounters the cluster. As more particles are simulated like this, a fractal is formed. One measure of the produced cluster is its fractal dimension.

I.A. Fractals

Fractals are objects for which the topological dimension[4] is not equal to their fractal dimension[5]. Fractals have a non-integer dimension and exhibit a property called self similarity, whereby scaled segments of the fractal closely resembles its larger structure.

Conventionally, we are experienced with objects whose dimension (d) is an integer (e.g a 1D line or a 2D square) where the object scales with 2^d. To demonstrate, doubling the side length of a square increases its area by 4 which is 2^2, thus, the dimension of a square is 2. One could easily compare to doubling the radius of a sphere which causes the volume to increase by eight, hence $d = 3$; or similarly to a line which doubles in length, $d = 1$.

Unlike these objects, the calculated dimension of a fractal is not an integer. There are numerous methods which can be employed to determine a fractal's dimension. One method is box counting, where the fractal is observed on successively smaller grids of boxes and the number of boxes containing a fragment of the fractal counted (see appendix B). Alternatively, another method counts the number of points, N, of size a required to construct an object which has a radius of R. The fractal dimension in this case is

$$N = \left(\frac{R}{a}\right)^d, \tag{1}$$

where d is the fractal dimension[6]. These methods will be used to measure the prodcued DLA clusters.

II. DLA SIMULATION

A simulation was ran in C++ which simulated the DLA system described in section I. Code was provided by A.Souslov and V.Rimpilainen[6]. A new simulation was created with a few key differences to their previous method. These differences will be explained in section II.B.

II.A. Previous Method

The simulation provided by A.Souslov and V.Rimpilainen creates a seed particle at the origin of a grid. Particles are then created one at a time which undergo random steps in the x or y direction. When the particle encounters a clustered particle it ceases to move and joins the cluster, at which point a new particle is

created. As described in Witten and Sander's paper[3] the simulation runs quicker[6] by generating particles on a circle at a fixed distance from the cluster. Likewise, the simulation is also sped up by resetting any particles who exceed another circle at a further distance (r_{kill}) from the cluster (see figure 5 in appendix D)[6].

Finally, the fractal dimension is calculated from the number of particles (N) forming the cluster and the radius of the furthest clustered particle (r_{max}) from the origin. From equation 1 the fractal dimension is found from the gradient of the line of best fit connecting $\ln(N)$ to $\ln(r_{max})$. According to equation 1, these are related by

$$\ln(N) = d\ln(R) + \ln(\beta), \tag{2}$$

hence, the gradient should measure the fractal dimension. The simulation was ran numerous times, each time creating a different fractal, and the dimension finally determined from these values.

Modifications were made to the code decreasing the walker sticking probability from its original value of 1.0. Instead of every 'collision' with the cluster aggregating, this probability determined whether walkers would stick. Particles which did not stick kept on walking. Simulations revealed that the sticking probability and kill radius influenced the fractal dimension. In subsequent investigations these were left at their default values provided in the original code.

II.B. New Method

A new simulation was created to simulate the system. One change was that the size of the simulation could be easily changed. The boundaries of the system could also be modified so that particles bounced off of the boundary, or made periodic so that particles which tried to leave the right hand side of the system reappeared on the left. In the previous method the boundary was never a concern since the kill circle limited walkers to the center of the grid. Unless stated the periodic boundary was used, although, no difference was measured in the fractal dimension under both variations. In addition, the new simulation allowed for more control over the seed particles (see fig). For the simulations explored in this paper only one central seed particle is used, as in the previous method.

Under the conditions stated, one would expect the two simulations to produce the same fractal since neither differ in the growth mechanism nor properties of the system. Having verified this conclusion, a final change was made to the simulation of the walker particles. Under the new method, walkers could either be generated individually until they contact the cluster (as already explored in section II.A by A.Souslov) or all the particles could be generated and diffuse simultaneously[7]. As such, a new property was introduced into the system, the area density of walker particles, ρ. The system was filled with particles at a density ρ, in random positions. On contact with the cluster, the particle would stick and then a new particle would be created at a random position. If the new position was on or contacting the cluster, the particle was abandoned. By creating new walkers when the particle joins the cluster, and discarding particles inside the cluster the density was kept constant throughout the simulation to within 2% of the specified density.

III. MEASURING THE FRACTAL DIMENSION

There were two different techniques which could be used to measure the clusters fractal dimension. The first, referred to as radial fractal dimension, is implemented by applying equation 2 to the cluster, using the distance of the furthest point from the origin as the measure of the radius[2,5,6]. This method is commonly used in DLA[2,3,5].

An alternative method is box counting[5,8] which again uses scaling, but is particularly useful when the radius of the system is not easily assessed.

In the following (sections III.A and III.B) a comparison of the two techniques will be made and assessed for use in further investigations.

III.A. Radial Fractal Dimension

Using the provided code by A.Souslov and V.Rimpilanen, a DLA cluster is grown to 3500 particles. The maximum radius (r_{max}) and number (N) of cluster particles is written to a `.csv` file. A linear fit of the logarithm of these values according to equation 2 is applied. Based on the described measure of the fractal dimension, the cluster is found to have a fractal dimension of 1.7553 ± 0.0231.

Using the same technique, the fractal dimension of a cluster using the new simulation code, where particles are singularly generated, had a fractal dimension of 1.7568 ± 0.0159.

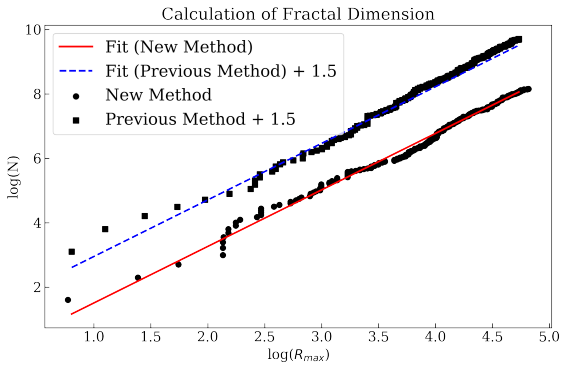


FIG. 1: Plot used to perform a linear fit to the radial data. The values for the original method has been offset by 1.5 units to increase the clarity of the diagram. The fractal dimension of the cluster is obtained from the gradient.

These measurements are a promising indication that the new simulation properly implements the DLA method. Within the measurement uncertainties both simulations produce the same fractal dimension for singularly generated particles.

The uncertainties in the measurements above were obtained from the co-variance matrix of the linear fit, which was performed using the `polyfit` function provided with the widespread `numpy` package in python. The simulation was ran a minimum 5 times, and these results used to generate the values above.

Having shown that the different simulations have the same fractal dimension under this method, box counting was then used.

III.B. Box Counting Fractal Dimension

Box counting, as the name implies, counts the number of occupied boxes when the fractal is placed on a grid. The size of grid boxes is then reduced and the number of occupied boxes once again counted. The number of occupied boxes scales with,

$$d = \lim_{\epsilon->0} \frac{\log N(\epsilon)}{\log 1/\epsilon}, \tag{3}$$

where d is the fractal dimension, N the number of occupied boxes as a function of the scale of the boxes ϵ[5,8]. As in the radial method, a linear fit is used for grid of 1 to 30 boxes and the fractal dimension obtained from the gradient.

Unfortunately, due to the output style of the previous method, the fractal dimension could only be calculated using box counting for the new simulation code. However, the previously made measurement using the radial method had demonstrated that within the measurement uncertainties the DLA clusters grown in the two simulations should have the same dimension.

III.C. Comparison

Box counting has the advantage of a lower uncertainty than the radial method. Using box counting, the simulation had a fractal dimension of 1.716 ± 0.007. Again, the uncertainty specified here was based on the uncertainty in the linear fit of data from a minimum 5 simulations. Indeed, the value calculated is consistent with the published 1.71[2,5].

By using box counting to asses the fractal dimension, the measurement uncertainty was halved ($\approx 0.016 \rightarrow 0.007$), as opposed to the the radial method. It is proposed that this systematic miscalculation is a consequence of the measurement of the cluster radius and finite cluster size. In addition, there was a systematic error causing the radial dimension to be higher than the widely accepted value. In order to reduce the error in the radial fractal dimension, clusters with a very large radii must be simulated[6]. However, as the cluster grew the radial growth rate decreased, consequently, the simulation time for such clusters became unfeasibly large.

The new method was quicker to run, allowing for much larger simulations to be created. As such, larger simulations, and subsequently lower uncertainties, could be performed. Importantly, box counting required a sufficient number of particles in the cluster so that, on the scale of the box grid, the fractal always appeared continuous. As the box size approached the scale of points, the count of occupied boxes saturates and the technique breaks down. Before this limit, box counting had a lower uncertainty than its radial counterpart.

IV. INVESTIGATION

Two main lines of enquiry were explored for the growth of the system; how the probability of a particle sticking to the cluster affected the growth of the cluster; and how the density of surrounding particles influenced the clusters growth.

Initially, the effect of the sticking probability was determined.

IV.A. Sticking Probability

The effect of the sticking probability was implemented by generating a random floating point number between 0 and 1. If this number was less than the user defined sticking probability the particle would aggregate onto the cluster, otherwise it would keep on walking. By allowing the particle to keep walking it now had the option to 'diffuse' towards the cluster center. Under this circumstance, one would expect to create a denser cluster with a higher fractal dimension.

Visually, the shrinkage and cluster filling was observed in both simulations. The improved accuracy of the box counting technique, and faster simulation times meant that measurements were conducted using the new method and box counting.

IV.A.1. Results

As expected, the growth rate of systems with lower probabilities was much slower than when all particles stick ($p = 1.0$). This result is understood as the expected number of 'collisions' must be far greater in order for a particle to stick.

Systems with a lower sticking probability were smaller relative to the number of particles contained in the cluster. From figure 2 it can be seen that a log-log plot would reveal an increasing radial fractal dimension for systems with a decreased sticking probability.

Using box counting, clusters with sticking probabilities matching those in figure 2 were grown. Indeed, these results verified the ansatz, that decreasing the sticking probability increased the fractal dimension. In fact, the fractal dimension tends to a value of 2.0, an unsurprising result since a cluster with no gaps would be a two-

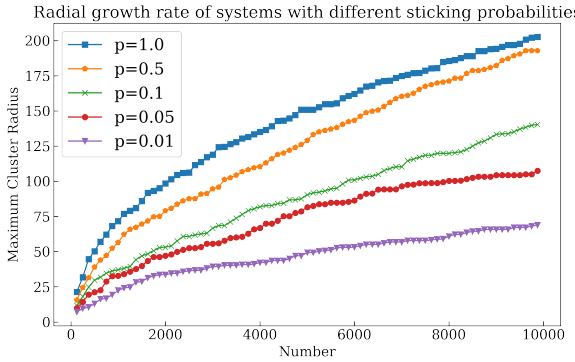


FIG. 2: Clusters with a lower sticking probability were smaller for the same number of particles. Simulations were generated in 14.42, 17.11, 24.97, 28.11 and 40.93 seconds in order of decreasing probabilities.

TABLE I: Decreasing the sticking probability increases the fractal dimension which tends towards a two dimensional object.

STICKING PROBABILITY	FRACTAL DIMENSION	(±)
1.0	1.707	0.011
0.5	1.730	0.022
0.1	1.806	0.005
0.05	1.865	0.025
0.01	1.941	0.039

dimensional circle. Running the simulation, it was evident that systems with a lower sticking probability did tend towards the two-dimensional case of a filled in circle (see figure 3). Measurements in table I verified these results; as the sticking probability decreased, the dimension tended towards 2.0.

IV.B. Density

The DLA simulation was then modified slightly. Instead of generating particles individually, a set number of particles were generated at $t = 0$, where t is the simulation time. At each time step every particle took a random step as specified section II.B.

These walkers did not interact with each other - a condition which was true for the singularly generated particles who had no experience of those subsequently generated. In the low density limit, this condition was assumed to be a good approximation - as walkers are too sparse to contact one another (at a density of 0.1% walkers could take an average of 60,000 steps without interacting - see appendix). The density of walkers was given by the equation

$$\rho = \frac{n}{wh}, \tag{4}$$

where n is the number of walkers, w the width of the grid the walkers are contained in and h the height. Unless otherwise stated, the width and height of the system were 500 units by 500 units.

IV.B.1. Results

DLA clusters were grown as a function of the density of walkers on the grid. In these simulations the sticking probability was kept constant at 1.00 so as not to skew the results, by causing all of the fractal dimensions to tend towards 2.0. Table II contains the calculated fractal dimension for walker particles at different densities over 10,000 time steps. For densities less than 1%, within the measurement uncertainty, the same dimension remains at the literature value. At 5% and beyond, an increase in the fractal dimension is measured, with the fractal dimension, again, tending towards 2.0. Given that the fractal dimension is unchanged, it is reasonable to assume that for low densities ($< 5\%$) the process remains 'diffusion limited'. Beyond this density, the cluster 'explodes' outwards; growing by accumulating particles in neighbouring sites rather than waiting for them to diffuse onto the cluster.

TABLE II: Increasing the walker density increases the fractal dimension, which tends towards a two dimensional object.

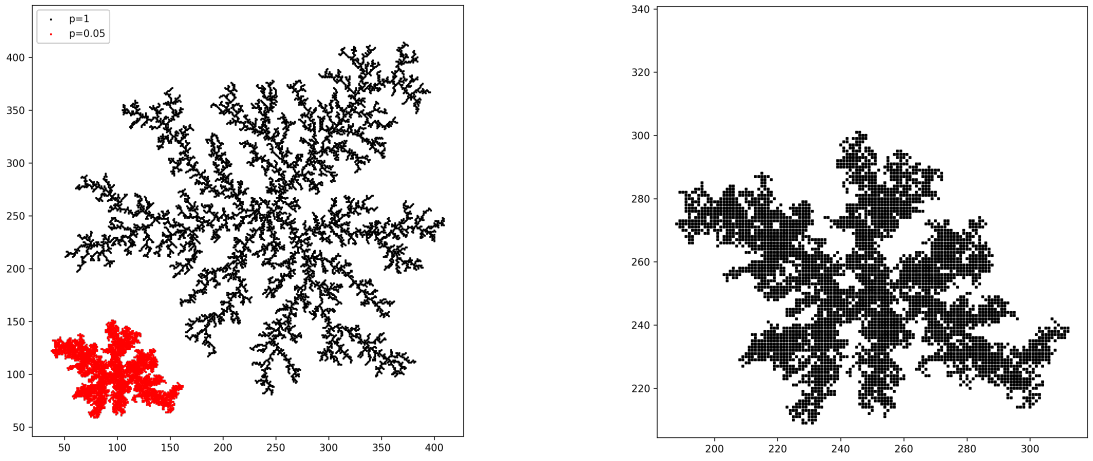
Walker Density (%)	Fractal Dimension	(±)
0.1	1.690	0.010
0.5	1.706	0.006
1	1.706	0.006
5	1.735	0.009
10	1.799	0.006
25	1.935	0.001
50	1.957	0.030

V. DISCUSSION

Section III.C found box counting to be a more accurate method of calculating the fractal dimension.

When the sticking probability of walkers is explored, as expected, a probability of 1.0 yields the literature value. Decreasing the sticking probability increases the number of times a walker must collide with the cluster resulting the the cluster being 'filled in'. Measurements of the simulation corroborate this theory and it was confirmed that a decreasing sticking probability causes the fractal to fill in - giving a dimension closer to that of a two dimensional object.

The results in section IV.B.1 can be interpreted by considering how the cluster grows. In order for the process to remain diffusion limited, there must be fewer particles on the rim of the cluster, than particles diffusing onto the cluster. In a purely diffusion case based on singularly generated particles, there will be a maximum of one particle aggregated onto the cluster at each time step, as was the case with the code provided by A.Souslov[6]. An equation has been derived (see appendix C), based on this condition, relating the density to the number of par-



(a) (b)

FIG. 3: Simulations of DLA clusters with sticking probabilities of 1.00 and 0.05. The latter is offset and smaller in red for visibility, with a scaled up version plotted in figure 3b.

ticles in the cluster,

$$\rho \leq \frac{1}{2\pi\sqrt{\frac{1}{6}N}}, \tag{5}$$

with the density of particles ρ and number of cluster particles N.

Based on this estimate, for a typical cluster size of 1000 particles[9] the system will remain diffusion limited for densities less than 1%. Remarkably, this is in perfect agreement with the result obtained in table II. Alternatively, one could probe equation 5 by measuring the dimension as the cluster grows, as is the case in figure 4. Once again, equation 5 proves itself to be an accurate representation of the system. At a density of 0.02 a cluster of 500 almost particles should remain in diffusion limit. Once the cluster exceeds this critical size its growth will be dominated by the occupancy of nearby particles. As expected, figure 4 demonstrates this size dependence. Until 500 particles the fractal dimension remains at the literature value of 1.71[2,3,5,10], beyond this limit the fractal dimension begins to diverge from the diffusion value. In practice, figure 4 demonstrates that clusters can be grown to almost twice this size before the fractal dimension changes significantly.

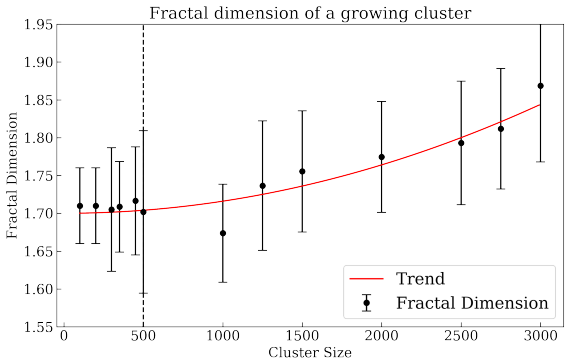


FIG. 4: A cluster grown at a density of 2%. At 500 particles the growth will be dominated by particle occupancy. Indeed, once the particle reaches this critical size the fractal dimension begins to increase, tending towards 2.

Of note is the size of error bars in figure 4, before 500 particles there is relatively few data points in the linear fit used by the box counting algorithm (as boxes must remain much larger than data points) giving rise to large uncertainties in the measurement despite the values not significantly deviating from 1.71. Beyond this critical cluster size, error bars are relatively large due to the spectrum of fractal dimensions in the cluster - at the centre there are 500 particles with $d = 1.71$ but further out the fractal dimension is higher. The error is a consequence of this non-linear change.

VI. CONCLUSION

It has been shown by simulations that the DLA process proposed by Witten and Sander[3] produces a fractal with a dimension consistent with the literature value of 1.71[5]. Further modelling, changing the probability of a walker joining the cluster causes the fractal dimension of the DLA cluster to tend towards 2.0. Yet more investigation into the density of walkers, rather than singularly generated particles, gave an equation which can be used to determine the density of walkers for which the process will remain diffusion limited. Beyond the limit, the dimension, again, tends towards two, caused by the outward growth of the cluster being dominated by neighbours rather than diffusion onto the cluster. Box counting provided a more accurate robust method for calculating the fractal dimension of clusters.

Appendix A: References & Footnotes

[1]R. Rennie and J. Law, "diffusion limited aggregation," (2019).
[2]P. Meakin, S. Tolman, and A. Blumen, "Diffusion-limited aggregation [and discussion]," Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences **423**, 133–148 (1989).
[3]T. A. Witten and L. M. Sander, "Diffusion-limited aggregation, a kinetic critical phenomenon," Phys. Rev. Lett. **47**, 1400–1403 (1981).
[4]Dimension of space the fractal exists in.
[5]J. Feder, *Fractals*, 1st ed., Physics of Solids and Liquids (Springer US : Imprint: Springer, New York, NY, 1988).
[6]A. Souslov and V. Rimpilainen, *PH30056 Coursework*, University of Bath (2021).
[7]Walkers could also travel a cell diagonally which wasn't possible in the previous method.
[8]S. Crampin, *PH30055 Worksheet Assignment 2*, University of Bath, 1st ed. (2020).
[9]On a grid 500 by 500.
[10]P. Meakin, "Progress in dla research," Physica D: Nonlinear Phenomena **86**, 104–112 (1995), chaos, Order and Patterns: Aspects of Nonlinearity - @'The Gran Finale@'.

For more information please visit `http://edwardwebster.me/DLA`
All files can be accessed on GitHub `https://github.com/edwardwebster/PH30056-Labs/tree/master/Coursework\%201`

Appendix B: Box Counting

Box counting counts the number of occupied boxes where a fractal is placed over a grid of boxes. The scale of boxes is reduced and the count repeated, from this the fractal dimension can be calculated. Pseudo code for box counting is contained below:

```
function boxcount(data, number of boxes):

    boxes[n, m] = 0
    width = width of boxes

    for all data:
     [i, j] = np.trunc(data/min(data)-width)
        box[i, j] = 1

return sum(boxes)
```

The data is divided into the specified number of boxes. The minimum is taken from each data point and the box this point belongs to found. For all data points occupied boxes are found and the sum of occupied boxes is the box count. From a linear fit of the scale and number of filled boxes the dimension is found.

Appendix C: Density Diffusion Limit

For the growth process to remain diffusion limited, section V concluded that the number of walkers on the circumference of the cluster must be less than the purely diffusion case for which there can only be a maximum of one particle diffusing on to the cluster each time step. The number of available connection points is proportional to the radius of gyration[5] by $2\pi\sqrt{< R_G^2 >}dr$ which is the area of a two dimensional shell at $\sqrt{< R_G^2 >}$ with width dr. For diffusion, the number of particles on this shell must be less than one. Thus, the following estimate is produced for the diffusion limiting case,

$$\begin{aligned} \#\text{ on cluster rim} &\leq 1 \\ \rho \cdot 2\pi r dr &\leq 1, \\ \rho &\leq \frac{1}{2\pi < R_G^2 >^{1/2} dr}, \\ \rho &\leq \frac{1}{2\pi\sqrt{\frac{1}{6}N}}, \end{aligned} \tag{C1}$$

where ρ is the density of particles, $< R_G^2 >^{1/2}$ the radius of gyration, N the number of particles in the cluster and $dr = 1$, which is the distance at which particles aggregate onto the system. The radius of gyration is used to measure the radius of r of the cluster, it can be expressed in terms of the number of particles in the system[5] as $< R_G^2 >= \frac{1}{6}Nb^2$; which can be simplified to $\frac{1}{6}N$ as the step size (b) is equal to 1.

Appendix D: DLA Simulation by Witten and Sander

The following image from Meakin's 1995 paper shows the addition, kill and maximal radius circles of the DLA simulation used by Witten and Sander.

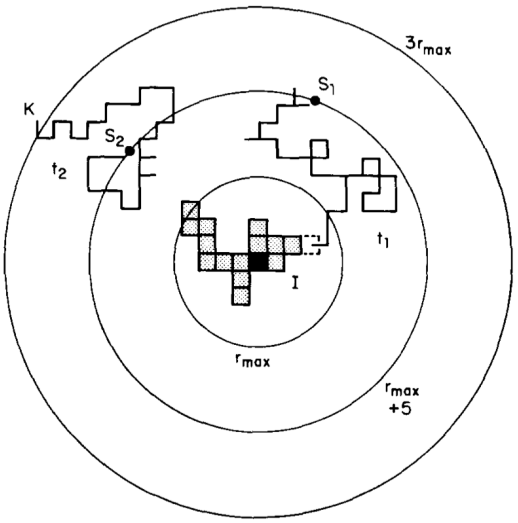


FIG. 5: Schematic of simulation used by Witten and Sander. Particles are created at $r_{max} + 5$ and killed at $3r_{max}$. Particle s_1 is shown joining the cluster and s_2 being killed. Image from Meakin 1995[10].

Appendix E: Simulated DLA Fractals

Below is a series of DLA fractals of interest which could not be contained in the main body of the report. Each contains a brief description and a calculated fractal dimension.

Unless otherwise stated, all clusters are grown on a 500 by 500 periodic grid, with a sticking probability of 1.0. 5000 particles are simulated for 10,000 steps.

1. Multiple Seeds

The figure below shows a cluster produced with seeds in the lower and upper corners. Generated for 7500 particles after 80,000 time steps with non-periodic boundaries. The figure shows the effect of boundaries on the pattern.

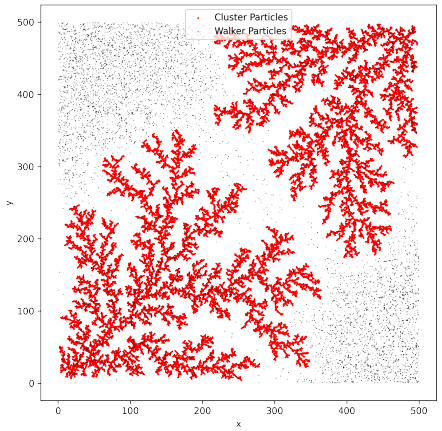


FIG. 6: System grown with seeds at (20, 20) and (480, 480) on a 500 by 500 grid.

Interestingly, the density of walkers does not appear to be constant, between the two clusters it is lower. This is an indication that the system is not in the low density limit. Further experimentation could have ran the system for longer in the low density limit.

Because there are two clusters the radial fractal dimension method is incompatible with this system as there are multiple objects. Box counting proves use full in calculating the fractal dimension. The fractal dimension here will be affected by the boundaries, the density, and having dual clusters. Using box counting the fractal dimension was calculated to be 1.77 ± 0.06.

2. Density Growth

Clusters can be grown at low or high densities, as described. In the low density case below a cluster is grown at a density of 4×10^{-5} particles per square for 1,000,000 time steps (which was more than required as the cluster is completely formed i.e there are no left over particles). The fractal dimension is 1.72 ± 0.01. The next figure shows a cluster grown at a density of 0.04 particles per square unit (10 times higher than the previous figure) for 20,000 time steps. This density allows the cluster to explode outwards. When simulating the high density system, the growth rapidly accelerates, predicted by 5. The

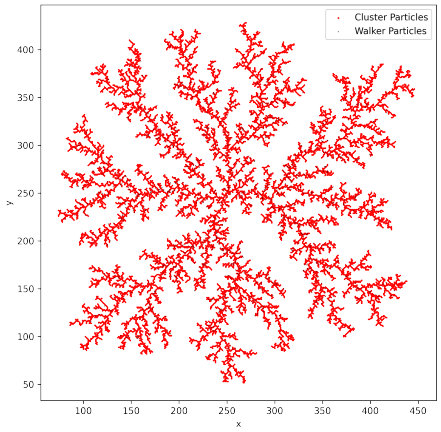


FIG. 7: System grown at low density

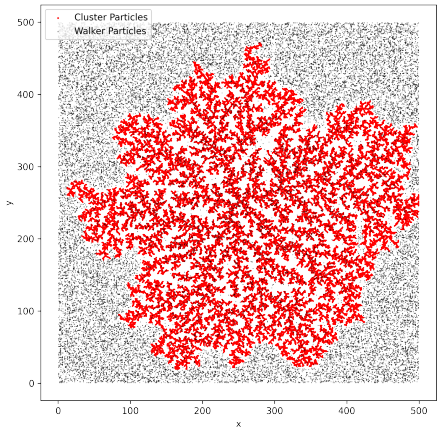


FIG. 8: System grown at high density

fractal dimension is calculated to be 1.84. This is higher than the low density case. There are far more particles outside of the cluster than in the low density limit, this is a consequence of the rapid outward growth. Instead of diffusing onto the cluster particles cant move out of the way before they are aggregated.