Thermodynamics and Diffusion Limited Aggregation

Candidate Number: 21594
Department of Physics, University of Bath, Bath BA2 7AY, United Kingdom

Abstract. Abstract goes here

Todo list

Preface

Although the coursework was initially presented as a C++ project, I took the liberty of rewriting the DLA system in a programming language called Google Go. The motivation for this is Go more easily supports high concurrency. This means that instead of simulating 1 cluster at a time, 100 different clusters can be simulated simultaneously in different threads. To support this high level of concurrency, the results were generated by running the code on a 32-core virtual server. The code can be obtained by visiting https://github.com/hcoplestone/DLA.

1. Introduction and Simulation Method

Diffusion Limited Aggregation (DLA) is a theory that models the process of how clusters of particles grow, in cases where growth is driven primarily by diffusion. [1]

In the DLA method used in this paper, a stationary seed particle is placed at the centre of a regular square lattice. This seed particle defines the origin of our system, as shown in Figure 1. A

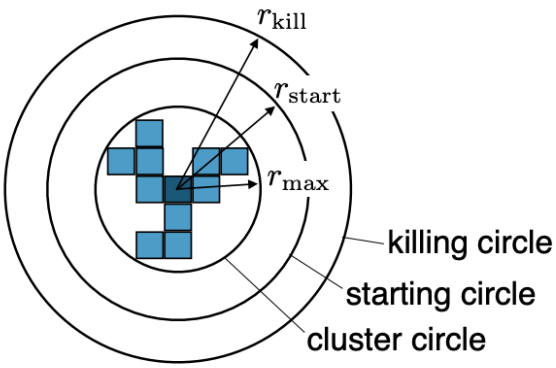


Figure 1: "Diagram of the circles used in the DLA code. The initial particle is shown in dark blue, and all circles are centred on this particle. There are three circles which indicate the approximate cluster size ('cluster circle'), the locations at which particles are introduced to the system ('starting circle'), and the points at which particles are removed from the system, to prevent them from wandering too far from the cluster ('killing circle')." Diagram and caption lifted verbatim from [2].

particle is then added to the system at a radius r_{start} from the origin. This radius is computed such that each new particle is added at a radius greater than the radius of any stationary particle in the system. Diffusion limited transport is driven by Brownian motion [3], a random process, so the new particle is made to undergo a Markovian random walk through the system. If the particle moves to a cell on the lattice that is horizontally or vertically adjacent to a stationary particle, the particle is stuck to the grid cell with a sticking probability p_{stick}. If the particle moves too far away from the cluster, as defined by a radius r_{kill}, the particle is removed from the system. Once a particle is stuck to the cluster or killed for 'walking' too far away, a new particle is added on the start circle and the process is repeated. The simulation is terminated when the border of the cluster approaches the edge of the lattice or when the total number of particles in the cluster reaches a predefined limit.

In this paper, it is tested to see if the maximum number of particles used in a DLA system affects the fractal index of the generated cluster. Enquiry is also made into how fractal dimension depends on the sticking probability d_f, as this links to the thermodynamics of physical systems that can be modelled using DLA.

2. Method

2.1. Random Walks and Ensemble Averaging

To simulate the Brownian motion of diffusing particles, DLA simulations have free particles undergo a random walk. For each iteration, the direction a particle moves in is parameterized by a discrete random variable $D \sim \mathcal{U}\{0,3\} \cap \mathbb{Z}$, with each value of D corresponding to one of the particle's degrees of freedom - 2 horizontal and 2 vertical. The issue with this is that the sequence of random numbers generated by the random number generator algorithm used in the DLA simulation is only 'pseudo-random'. For a given random number generator seed, the same sequence of numbers will always be generated. This may bias the results of the simulations. To mitigate this, an ensemble of systems are simulated independently, each with a different random number generator seed. For a given measurement $\xi(t)$, an ensemble average $\overline{\xi(t)}$ is calculated by averaging measurements from each of these n systems $\{i\}_1^n$, where i represents a specific simulated system:

$$\overline{\xi(t)} = \frac{1}{n}\sum_{i=1}^{n} \xi_i(t) \tag{1}$$

2.2. Determining the Fractal Dimension of DLA Aggregates

DLA clusters are fractal objects. This means their geometric structure can be described by a measure called 'fractal index', d_f. For a DLA system, the fractal dimension can be defined by [2]

$$N_c(r_{max}) = (\alpha \cdot r_{max})^{d_f} + \beta \tag{2}$$

Taking logs of both sides and differentiating with respect to $\ln r_{max}$ yields

$$\frac{d(\ln r_{max})}{d(\ln N_c)} = \frac{1 + \beta/(\alpha \cdot r_{max})^{d_f}}{d_f} \tag{3}$$

which in the limit of large r_{max} gives

$$\lim_{r_{max}\to\infty} \frac{d(\ln r_{max})}{d(\ln N_c)} = \frac{1}{d_f} \tag{4}$$

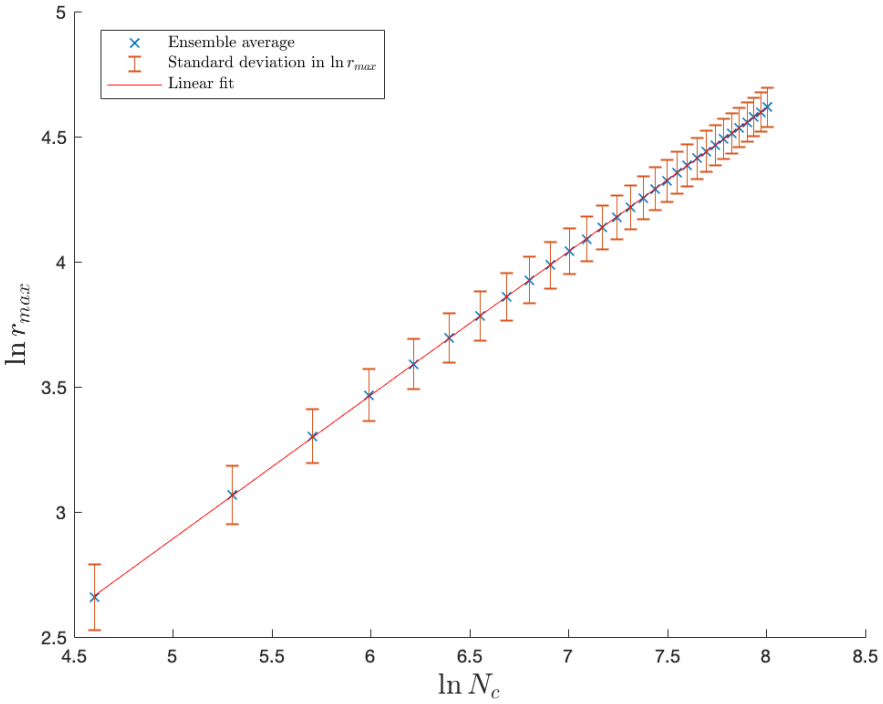


Figure 2: Natural log of cluster radius, r_{max}, as a function of the natural log of the number of particles in the cluster, N_c. Data points represent average over 1000 subsystems using equation 1. Error bars represent the standard deviation in the values of $\ln r_{max}$. Application of equation 4 yields $d_f = 1.74$.

2.3. Sticking Probabilities

DLA systems can be setup so that the sticking probability p_{stick} is less than 1, indicating that a particle may sometimes collide with a cluster and recoil. This is useful when studying systems with a high thermodynamic temperature, for example. To achieve this, when the system determines that a particle has moved into a grid cell where there is the possibility of 'sticking', a random number p is sampled from a continuous uniform distribution $P \sim \mathcal{U}\{0, 1\}$. If $p \leq p_{stick}$ then the particle is marked as stationary and the system proceeds to add a new particle. In the case $p > p_{stick}$, the direction of the particle is reversed and moved one grid cell.

3. Results

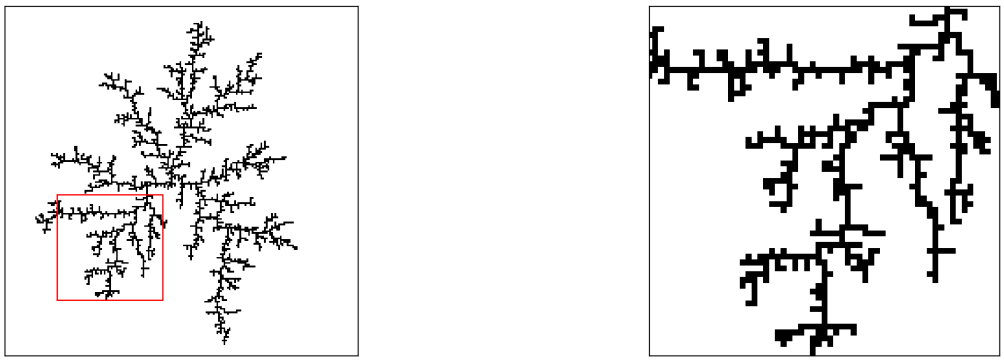
3.1. Determining the Fractal Dimensions of DLA Aggregates

Figure 2 shows the ensemble average of the natural log of the cluster radius as a function of the natural log of the number of particles in the DLA cluster, averaged over $n = 1000$ independent systems with different random number generator seeds. Application of equation 4 yields a fractal dimension for 2D DLA systems of $d_f = 1.74$.

Need to calculate error

3.2. Self Similarity

Figure 3 shows graphical representations of the results of a DLA simulation with 3000 particles. 3 (a) shows the entire cluster and (b) shows the bounded area from (a) magnified. Observe how all the major branching parts in Figure 3 (b) have exactly two child branches - one emerging downwards and one emerging to the left. This demonstrates the fractal, or self-similar, nature of the DLA model.



(a) Entire DLA Cluster (b) Magnification of branch

Figure 3: Graphical representation of a DLA cluster with 3000 particles. (a) shows the entire DLA cluster and (b) shows a magnification of the bordered section in (a).

4. Discussion

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5. Conclusion

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References

[1] T A. Jr Witten and Leonard Sander. Diffusion-limited aggregation, a kinetic critical phenomenon. prl, 47:1400–, 11 1981.

[2] V. Rimpilainen A. Souslov and R. Jack. Dla coursework assignment. Handout, 2019.

[3] Albert P Philipse. Brownian Motion : Elements of Colloid Dynamics. Undergraduate Lecture Notes in Physics. Springer International Publishing : Imprint: Springer, Cham, 2018.