The Effects of Simulation Parameters When Modelling Systems Using 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]

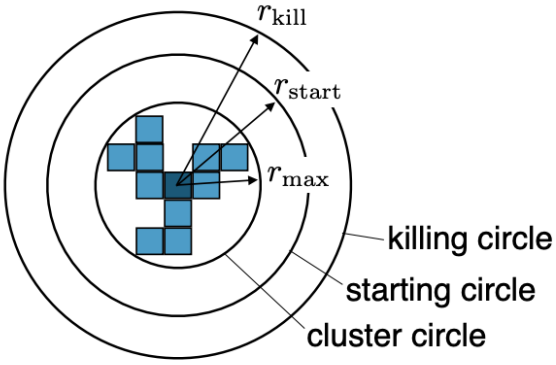

Figure 1: "Diagram of the circles used in the DLA code. The initial particle is shown in dark blue, and all circles are centred on this particle. There are three circles which indicate the approximate cluster size ('cluster circle'), the locations at which particles are introduced to the system ('starting 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].

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

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, we investigate whether the maximum number of particles used in a DLA system affects the fractal index of the generated cluster. We also investigate how fractal dimension depends on the sticking probability d_f, and link this to the thermodynamics of a growing system.

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:

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

Standard error $\sigma_{\overline{\xi}}$ can be used as a measure of how close the ensemble average is to the true value:

$$\sigma_{\overline{\xi}} = \frac{1}{\sqrt{n-1}}\left[\overline{\xi(t)^2} - \overline{\xi(t)}^2\right]^{1/2} \tag{2}$$

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 [2]. To determine the fractal dimension of each of the DLA clusters generated, a curve of the form

$$N_c(r_{max}) = (\alpha \cdot r_{max})^{d_f} + \beta \tag{3}$$

is fitted to the simulation data using a least squares fitting to optimise the free parameters α, β and d_f.

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 the 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 $p <= p_{stick}$ then we mark the particle

as stationary and continue to add a new particle to the DLA simulation. In the case $p > p_{stick}$, the direction of the particle is reversed and moved one grid cell.

Talk about method of varying sticking probability and calculating sticking probability. Include values for number of particles, and number of ensembles.

3. Results

3.1. Determining the Fractal Dimensions of DLA Aggregates

4. Discussion

bla

5. Conclusion

bla

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.