Pattern Formation in Diffusion Limited Aggregation and Reaction-diffusion Model

Scientific Compupting Assignment 2

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1 Introduction

Patterns, such as snowflakes, pigmentation in animals, branching trees and skeletal structures,etc. form in nature in a wide scale. Therefore, pattern formation has been explored by many papers. This report will explore the simulation of Diffusion Limited Aggregation and Reaction-diffusion model(Gray-Scott Model).

The first part of this report deals with Diffusion Limited Aggregation. It models the formation of patterns in nature, where diffusion usually dominates the transport. [1] Examples are the processes of matters irreversibly combines to form dust, soot, dendrites and other random objects diffusing and aggregating to the objects.[2] And this report will use two methods to simulate DLA: First is a growth model based on diffusing particles; Second is Monte Carlo simulation of DLA.

The second part deals with Gray-Scott model[3]. It tries to model the wide range of pattern formation in nature, such as pigmentation in animals. Gray-Scott model assumes a system of chemical reactions of U and V, both of which diffuse in the system, and also react with each other. The reaction rate at any point in space, is determined by the local concentrations of U and V. The reactions are:

$$\begin{aligned} U + 2V &\rightarrow 3V \\ V &\rightarrow P \end{aligned} \tag{1}$$

U is continuously fed into the system. It then reacts with V to produce more V. V spontaneously decays into P, an inert product. The resulting reaction–diffusion equations can be formulated as follows:

$$\begin{aligned} \frac{\partial u}{\partial t} &= D \bigtriangledown^2 u - uv^2 + f(1-u) \\ \frac{\partial v}{\partial t} &= D \bigtriangledown^2 v - uv^2 + (f+k)v \end{aligned} \tag{2}$$

, where U and V stands for the concentration of reactants U and V; Diffusion coefficients D_u, D_v , F and k are constants, f controls the rate at which U is supplied, and (f + k) controls the rate at which V decays. The first equation decides how quickly u increases in proportion to the Laplacian of U. The second term $-uv^2$ is the reaction rate, which is proportional to the probability of a collision of the reactants U and V, then thus proportional to the concentration of U times the square of the concentration of V, according to the Law of mass action. The third term F(1-u) is the replenishment

term. And for the second equation, the difference is the third term, which is the dimishment term for V.

For different value-combinations of f and k, a large variety of spatio-temporal patterns can be observed, with some result in asymptotically stable patterns, while others remain time-dependent. According to Pearson [3], with $\sigma = D_u/D_v = 2$ and initially a small (u, v) = (1/2, 1/4) square on an otherwise (1, 0) background with small noise, various patterns occur, ranging from regular to irregular steady patterns to chaotic patterns. As the parameter map Fig 1 Pearson concluded , some patterns such as $\alpha, \beta, \gamma, \eta$ are time-dependent, some patterns such as λ, θ, κ are time-independent, and pattern ε is chaotic.

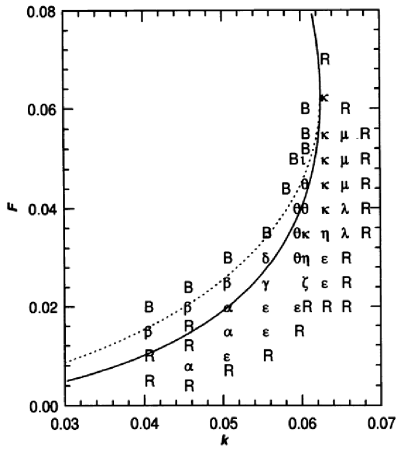

Figure 1: The map. The Greek letters indicate different pattern formations with the set of parameters at that position in parameter space, B and R indicate that the system evolved to uniform blue and red sates, respectively.[3]

Munafo [4] pointed out that "Pearson missed many types of patterns because he only used one starting pattern: a small (u, v) = (1/2, 1/4) square on an otherwise (1, 0) background." And he named those types as nu, xi, pi, rho and sigma, and further differentiated each pattern type by looking at key properties such as oscillation, spot shape, system-wide determination and local determination.

This report will explore Gray-Scott Model in two dimensions for various parameter combinations adopted by Pearson, with finite difference method and periodic boundary conditions, and show some of these patterns. Python3.4 will be used for all the simulations.

2 Method

2.1 Diffusion Limited Aggregation

2.1.1 Growth Model based on Laplace Model

The idea of Growth Model based on Laplace Model is to build Growth Model based on the diffusing particles in a lattice domain, where the concentration modeled is the concentration of free walkers to be introduced in next section.

Rules are as follows: First the growth is started with a single seed, which is represented by a sink in a single lattice point at the bottom of the computational domain. The simulation system is started with the analytical solution for the diffusion equation $\frac{\partial c}{\partial t} = D \bigtriangledown^2 c$. And then DLA can be modeled by solving the time independent diffusion equation,i.e. the Laplace equation, in the domain. In this report, the SOR method is used. As the growth step is constructed in such a way that on average only one lattice site is grown to the object, the concentration fields will hardly change. Therefore, this report will start a new SOR iteration with the solution of the previous growth step. Third, those grids not belonging to the cluster but whose neighbor grids contain at least one grid that belongs to the cluster are grouped as growth candidates. As Fig 2 shows, the black grids are parts of growth cluster, and the open circles are the growth candidates. Forth, a growth probability

$$p_g((i,j) \in cluster \rightarrow (i,j) \in candidates) = \frac{c_{i,j}^{\eta}}{\sum_{c(i,j) \in candidates} c_{i,j}^{\eta}} \tag{3}$$

is assigned to each growth candidate, and $c_{i,j}$ is the concentration of diffusing nutrients at grid (i, j). Next, the growth candidates are added to the cluster with above mentioned probability p_g. After this growth step, the diffusion equation is again solved with SOR method in the whole domain. This growing process is iterated for a large amount of steps, which means that the growth model is applied for equal amount of steps, each followed by the Laplace Model.

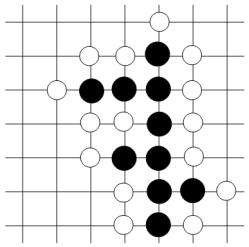

Figure 2: The location of growth candidates

Specifically for this report, various cluster patterns resulted from various η values, i.e. $\eta = 0, 0.5, 1, 1.5,\ 2,\ 4$ and 10, will be simulated respectively on a 200* 200 lattice domain. And the iteration amount is 1200 steps for the first four cases, and 800 for the last case.

The optimal parameter w values in the SOR iteration method for Laplace Model will also be explored for the case where $\eta = 0, 1,\ 2,\ 4$ and 10. While for cases where $\eta = 0.5$ and 1.5, w is set as 1, because the Eq 3 for growth probability requires the concentration values not less then 0. And SOR iteration sometimes will result in a concentration slightly less than 0 around the sink objects due to the accuracy tolerance.

2.1.2 Monte Carlo simulation of of DLA

The idea of Monte Carlo simulation of of DLA is to release random walkers on a grid, and letting them walk until they hit the cluster. When they hit, the walkers are stopped, become part of the cluster, and a new walker is released.

Rules are as follows:A walker is started the on a randomly chosen point on the top boundary of the domain. It moves in steps, which are randomly chosen to be one lattice point up, down, left, or right. If the walker reaches a cell neighboring the cluster, the walker is stopped there, so that the

cell with the walker becomes part of the cluster. And anther walker will be released at a randomly chosen point on the top boundary next time step. During the random movement if a walker walks out of the system on the top or bottom boundary it is removed and a new one created instead. If it walks across the left or right boundary, it should enter the system from the other side, as periodic boundary conditions were assumed in the horizontal direction.

This report will explore the pattern on a 300* 300 lattice domain with 2000 random walkers released.

Further, With variation of the sticking probability of the model the geometry of the clusters generated in the Monte Carlo simulations change. The sticking probability is the probability that the walker will stick to the cluster when it enters a cell which is a neighbor of the cluster. If it does not stick, the walk continues as normal. The walker is however not allowed to move into a site belonging to the cluster. Therefore, this report will simulate on various sticking probability, i.e. 0.25,0.5,0.75,1, to compare the the geometry of the clusters generated.

2.1.3 The Gray-Scott Model - a reaction-diffusion system

To implement explicit time-stepping procedure and finite difference method, reaction-diffusion equations in Eq 2 can be transformed into Eq 4 to calculate the non-boundary points, which is shown in orange in Fig 3, using forward difference approximation for $\frac{\partial u}{\partial t}$, and centered difference approximations for both $\frac{\partial^2 u}{\partial x^2}$ and $\frac{\partial^2 u}{\partial y^2}$.

Assume the system size is 200*200, for boundary points on c(x, y=0, t), c(x, y=199, t), c(x=0, y, t) and c(x=199, y, t) columns and rows, periodic boundary conditions are implemented by expanding the mesh points on (x,y) plane by one more column on the left side of the original matrix, resulting in a 201*201 simulation world, as it shows in Fig 3. So point values on first column are exactly the same as the last but one column, point values on the last column are exactly the same as the second column. And the same for the rows.

$$\begin{aligned} \frac{u_{i,j}^{k+1} - u_{i,j}^{k}}{\Delta t} &= D_u \frac{(u_{i+1,j}^{k} + u_{i-1,j}^{k} + u_{i,j-1}^{k} + u_{i,j+1}^{k} - 4u_{i,j}^{k})}{(\Delta x)^2} - u_{i,j}^{k} {v_{i,j}^{k}}^2 + f(1 - u_{i,j}^{k}) \\ \frac{v_{i,j}^{k+1} - v_{i,j}^{k}}{\Delta t} &= D_v \frac{(v_{i+1,j}^{k} + v_{i-1,j}^{k} + v_{i,j-1}^{k} + v_{i,j+1}^{k} - 4v_{i,j}^{k})}{(\Delta x)^2} + u_{i,j}^{k} {v_{i,j}^{k}}^2 - (f + k)v_{i,j}^{k} \end{aligned} \tag{4}$$

The parameters are as follows:

L=200;

$\Delta t = 1$;

$\Delta x = \Delta y = 1$;

Diffusion coefficients $D_u = 0.16$; $D_u = 0.08$;

Initial conditions are set similarly as Pearson [3]:

First, the entire system is placed in the trivial state(u=1,v=0). Then grids in the center of the system a small square, 7*7 in the center of 200*200 mesh point field, are perturbed to (u=1/2,v=1/4). Finally, random noise is added to break the square symmetry. The frequency of occurrence of noise is 1% for both U and V, and for U the concentration values are perturbed by adding a random number between -0.5 and 0, for V the concentration values are perturbed by adding a random number between 0 and 0.75. A typical example is shown in Fig 4. In order to figure the effect of noise, one pattern will be generated with initial conditions with and without noise for comparison.

f and k combinations:

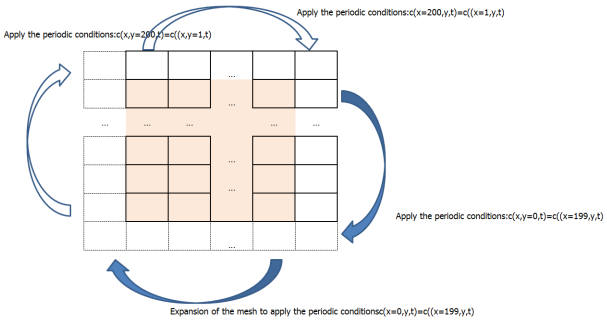

Figure 3: Application of periodic boundary conditions to the mesh grid field, with dashed grids indicate the expanded grids, and solid-lines grids indicate the original field.

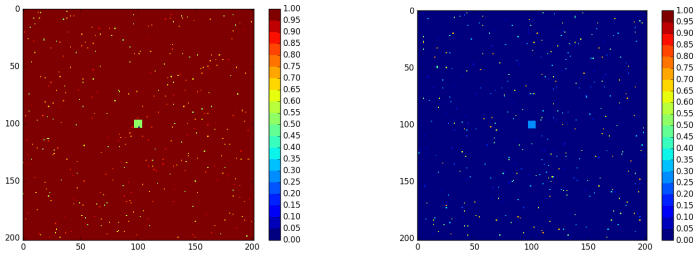

Figure 4: Initial conditions

1.f=0.035, k=0.06
2.f=0.016, k=0.05
3.f=0.03, k=0.057
4.f=0.034, k=0.065
5.f=0.01, k=0.041

Image exhibitions:

Python matplotlib library is used to show the concentration values for U and V. And "jet" color map is used to represent values from 0 to 1 with red to blue respectively for all the pattern images, i.e. in every image the colorbar is exactly the same as in Fig 4.

3 Results

3.1 Diffusion Limited Aggregation

3.1.1 Laplace Model with Growth Model

Fig 5 shows the iterations needed to reach the stopping condition with $\varepsilon = 10^{-5}$, for different w parameters in the SOR method. The errorbar represents one standard deviation of uncertainty, it shows that the uncertainty is large, while w=1.8 seems a relatively optimal selection.

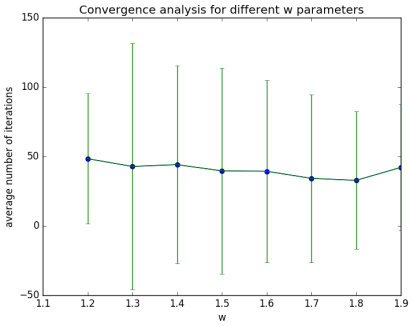

Figure 5: The iterations needed to reach the stopping condition with $\varepsilon = 10^{-5}$, for different w parameters in the SOR method

Fig 6 shows the clusters obtained with the diffusion equations. With η in Eq 3 for the calculation of the growth probabilities set to 0, 0.5, 1, 1.5, 2, 4, and 10, respectively, with iterations of 1200 for the first four clusters to add candidates into the cluster, and iteration of 800,200, and 50, respectively for the rest three clusters. The cluster structure changes from compact to diverging, and then when η is equal to 4 and 10, it can be observed that it resembles a lightning flash.

Note that in order to show the cluster image more clearly in Python 3.4, the mesh points belonging to the cluster, which should be a sink and whose concentration value is 0, are converted to value -0.2 after the whole cluster is formed.

3.1.2 Monte Carlo simulation of of DLA

Fig 7 are clusters obtained with the diffusion equation and Monte Carlo Simulation (sticking probability = 1) respectively. It can be observed that they are similar.

Fig 8 are clusters obtained by Monte Carlo simulation, with aggregation of 2000 particles on a square lattice of 300*300. With sticking probability set to 0.25, 0.75, and 1, the cluster structures change from compact form to scattered form. It is because for lower sticking probability, the walkers have to visit more places around the cluster before finally sticking. So, the probability of sticking to each of them is more equal than that of higher sticking probability.

3.1.3 The Gray-Scott Model - a reaction-diffusion system

This part will show the patterns resulting from the four pairs of parameter f and k combinations. Graphs are presented at another file **GSM graphs.pdf**, due to the memory limit in one Latex file.

1.f=0.035,k=0.06: For this pair of parameters, comparison is made with noise not added initially, shown in Fig 1, and randomly added initially, shown in Fig 2. As it shows in Fig 1, pattern is symmetric, and needs more time steps to diffuse over the field. It can be observed from Fig 2 (U concentration)and Fig 3 (V concentration) that this pattern is what Pearson [3] described as Pattern μ, which grow into stripes or branching structure, and stripes alter courses to avoid colliding.

2.f=0.016, k=0.05: It can be observed in Fig 4 and 5 that this pair of parameters is time-dependent and consists of fledgling spirals. And this is what what Pearson [3] described as Pattern α.

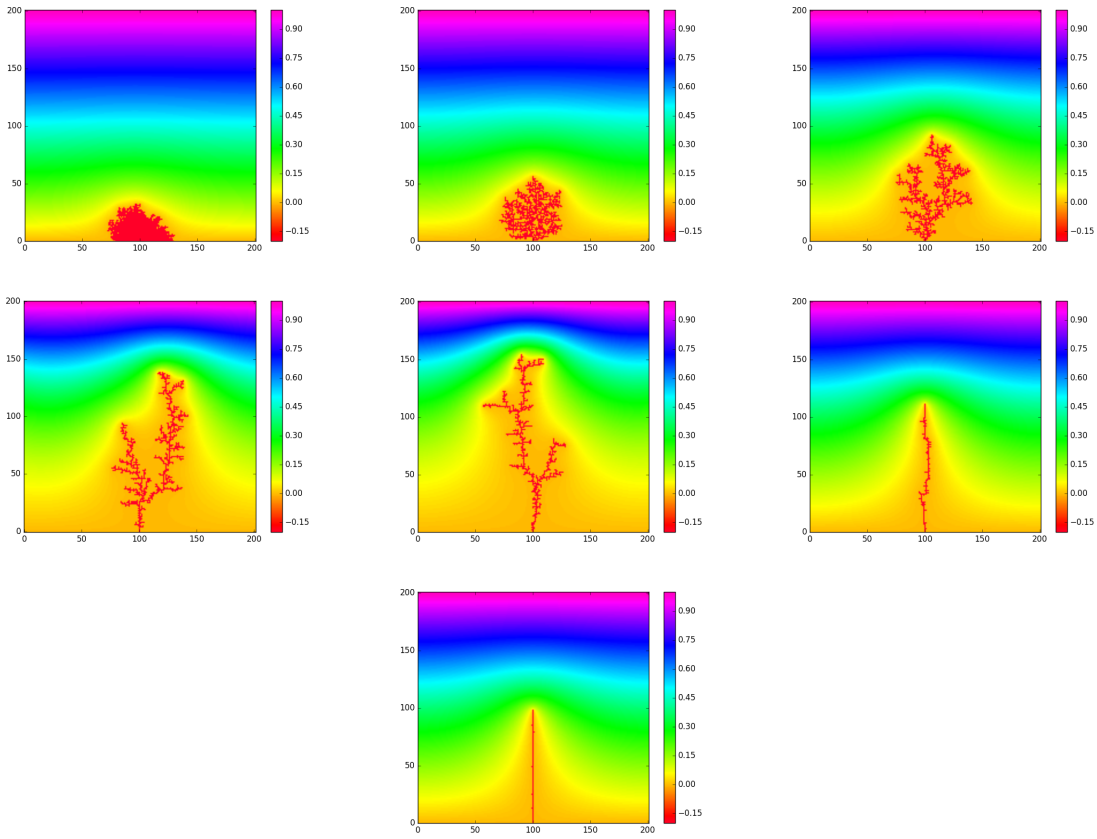

Figure 6: Clusters obtained with the diffusion equations. With η set to 0, 0.5, 1, 1.5, 2, 4, and 10, respectively.

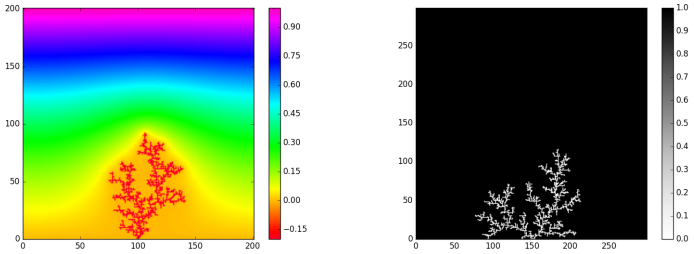

Figure 7: Comparison between clusters obtained with with the diffusion equation and Monte Carlo Simulation(sticking probability=1).

3. f=0.03 ,k=0.057 It can be observed in Fig 6 and 7 that this pattern is similar to the pattern resulting from (f=0.035,k=0.06) combinations in Fig 2 and 3. But it differs in that stripes stop when

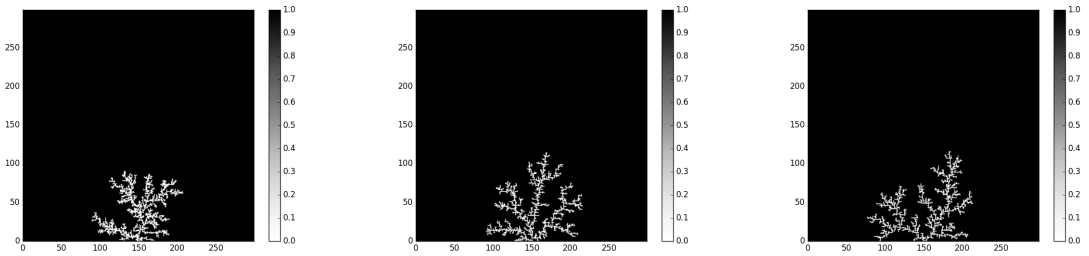

Figure 8: Monte Carlo simulation of of DLA, With sticking probability equal to 0.25, 0.75, and 1, respectively. All consist of aggregation of 2000 particles on a square lattice of 300*300.

colliding. And this is what Pearson [3] described as pattern θ.

4.f=0.034, k=0.065: It can be observed in Fig 8 and 9 that this pattern is filled with hexagonal grids, and time-independent after around 16000 time steps. And this is what Pearson [3] described as pattern λ.

5.f=0.01, k=0.041: It can be observed in Fig 10 and 11 that this pattern finally evolves into all red (for U) and blue(for V) state between 1000 and 2000 time steps.

4 Conclusion

This report explores the pattern formation of Diffusion Limited Aggregation by diffusion equation method and Monte Carlo Simulation, and of reaction-diffusion system by Gary-Scott Model. With variation of the parameters in the models, this report observes various interesting outcome patterns.

With the Diffusion Limited Aggregation by diffusion equation method, for $\eta < 1$ the cluster becomes more compact (with $\eta = 0$ resulting in the Eden cluster), and for $\eta > 1$ the cluster becomes more open. For Diffusion Limited Aggregation by Monte Carlo Simulation, the cluster becomes more compact when the sticking probability is close to 0, and for sticking probability close to 1, the cluster is more open. For the reaction=diffusion system, five type of patterns are simulated in the Gray-Scott model, with respect to five pairs of f and k parameters. The resulting patterns vary in the spatio-temporal space.

References

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