Scientific Computing Exercise Set 2

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I. Introduction

DIFFUSION limited aggregation (DLA) is a model which tries to model the growth of a cluster through diffusing particles. This can for example be applied to bacterial growth. Understanding DLA could help with understanding the growth of bacteria and allow for optimised processes where bacteria are involved. This report will look into two methods to simulate DLA, namely a diffusion method and a Monte Carlo method.

Additionally, this report will also explain the Gray-Scott model, which is a reaction-diffusion system. These systems are typically found in chemical reactions, where the chemicals react with each other and spread out over time.

II. Theory

TWO methods will be described in this section to model DLA. One method is through a diffusion field, which resembles the concentration of nutrients. At places where more nutrients are present the cluster has a larger probability to grow. The diffusion field is computed through a SOR method. The second method to model DLA is through a Monte Carlo method at which random walkers are released. The cluster will grow at the cite at which the random walker hits the cluster. Lastly, this section will also describe the Gray-Scott model, which describes a system of chemical reactions.

A. Solving the time independent diffusion equation

The diffusion equation describes how a substance spreads (diffuses) through an environment. If only the steady final state of the diffusion is of interest, the time independent diffusion equation can be used, which is given by

$$\nabla^2 c = 0 \tag{1}$$

where $c(x, y)$ is the concentration of the substance at coordinates x and y. Taking an environment that is a square with sides of length 1, the equation can be numerically solved by discretising the environment's x- and y-axes into N intervals of length $\delta x = 1/N$, so that the environment is represented as a lattice of size $N \times N$. Then the coordinates can be written as $x = i\delta x$ and $y = j\delta x$, where i and j represent the locations of the lattice sites, and so $i, j \in (0, 1, 2, ...N)$. Then the concentration at site i, j is defined as $c(i\delta x, j\delta x) \equiv c_{i,j}$.

The time independent diffusion equation can then be numerically solved using an iterative algorithm called *Successive Over Relaxation* (SOR). Since it is an iterative method, it becomes useful to use a superscript k to indicate the concentration of a lattice site after k iterations $c^k_{i,j}$. The SOR method iteratively calculates the concentration at a location using the concentrations of its neighbours through the formula

$$c^{k+1}_{i,j} = \frac{\omega}{4}(c^k_{i+1,j} + c^{k+1}_{i-1,j} + c^k_{i,j+1} + c^{k+1}_{i,j-1}) + (1-\omega)c^k_{i,j} \tag{2}$$

where ω is a parameter that dictates how much the method "compensates" for a change in value from its neighbours. The method is called over-relaxation for $\omega > 1$. This method uses a stopping condition to determine when the solution is accurate within a certain bound so that it can stop iterating. This stopping condition says that the method can stop iterating when

$$\delta \equiv \max_{i,j} |c^{k+1}_{i,j} - c^k_{i,j}| < \epsilon \tag{3}$$

where ϵ is a small number. This means that the solution is deemed accurate enough when the biggest absolute difference in a single iteration between the old and new concentration values of any lattice site (δ) is smaller than a set number ϵ.

This report looks at an environment with fixed boundary conditions $c^k_{i,N} = 1$, $c^k_{i,0} = 0$ and $c^k_{0,j} = c^k_{N,j}$ - so the concentration at the top row of the environment is always 1, at the bottom row always 0, and the x-direction always assumes a periodic boundary condition. For such an otherwise empty environment, the analytical solution of the time independent diffusion equation is given by

$$c(x, y) = y \tag{4}$$

which means that the concentration increases linearly with y.

B. Diffusion-limited aggregation

Diffusion-limited aggregation (DLA) is a model that simulates growth of particles by a random walk through

an environment, based on the diffusion field in that environment. The diffusion field represents the concentration of nutrients in every location. The growth cluster feeds on these nutrients and tries to grow towards areas with high concentrations. This report investigates two methods for implementing the DLA model.

1) Using diffusion equation: First, DLA can be implemented by simulating the actual diffusion of the nutrients through the environment, which is an $N \times N$ lattice. This is done by solving the time independent diffusion equation every iteration using the SOR method described in Equation 2 until the stopping condition is reached. The growth cluster starts as a single seed, located in one lattice point at the bottom of the environment. The cluster grows every iteration by selecting one random lattice site from a selection of growth candidates. A lattice site belongs to this selection if it is not yet part of the cluster, but neighbours a site that does belong to the cluster. A site's neighbours are the sites that are directly above, below, left and right of it. The cluster "chooses" a lattice site from the growth candidates, where a growth candidate's probability of being chosen is

$$p_g(i,j) = \frac{c_{i,j}^{\eta}}{\sum_{\text{growth candidates}} c_{i,j}^{\eta}} \tag{5}$$

where $c_{i,j}$ is the concentration of nutrients at that location and η is a parameter that determines the shape of the object. For higher values of η ($\eta > 1$), the cluster will have a higher preference to grow towards sites with a high concentration of nutrients - this results in a less dense cluster. $\eta < 1$ results in a more dense cluster, and when $\eta = 0$, all of the growth candidates have an equal growth probability p_g. This results in the *Eden cluster*.

After the cluster grows to a lattice site in an iteration, it "consumes" the nutrients there. This means that all of the lattice sites that are part of the object are sinks, and thus have a concentration $c_{i,j} = 0$. In this way, the growing cluster changes the diffusion field every iteration, requiring the time independent diffusion equation to be solved again, until the stopping condition is reached.

2) Monte Carlo simulation: Another method to simulate DLA is through the release of random walkers. These random walker will randomly move through a 2-dimensional grid of size N by N until they neighbour a cell corresponding to the cluster. When they reach the cluster they will become part of the cluster. This allows the cluster to grow. This method does not require the simulation of a diffusion field, as described in the diffusion method, which should speed up the simulation.

A drawback of this method is that η can not directly be incorporated in the random walker method. To simulate η a sticking probability p_s is added. This sticking probability is the chance that a random walker will stick against the cluster when it neighbours it. If the random walker does not stick it continues its path. The random walker is not allowed to pass through the cluster.

C. Gray-Scott model

In a reaction-diffusion system, multiple chemicals are present which both react with each other and diffuse through the environment, changing their concentrations at different locations. One such system is a Gray-Scott model. Here, two chemicals U and V are present which interact locally through the reactions

$$U + 2V \rightarrow 3V \tag{6}$$

$$V \rightarrow P \tag{7}$$

where P is a reaction product that does not interact with U or V. The concentrations of U and V, u and v respectively, can be described by the differential equations

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + f(1-u) \tag{8}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - (f+k)v \tag{9}$$

where D_u and D_v are the diffusion constants for the chemicals U and V respectively, f dictates the rate at which U is continuously fed into the system, and $f + k$ dictates the rate at which V spontaneously decays into P. Again, the environment can be discretised like was shown in section II-A, but since this solution is time dependent, time is also discretised into intervals δt with $t = k\delta t$ ($k \in N$). The concentrations of U and V at lattice site (i,j) and time $t = k\delta t$ are then indicated by $u_{i,j}^k$ and $v_{i,j}^k$.

Discretising Equations 8 and 9 using finite difference methods results in the iterative finite difference equations

$$u_{i,j}^{k+1} = u_{i,j}^k + \delta t * (D_u * \left(\frac{u_{i+1,j}^k + u_{i-1,j}^k + u_{i,j+1}^k + u_{i,j-1}^k - 4u_{i,j}^k}{\delta x^2}\right) - u_{i,j}^k {v_{i,j}^k}^2 + f(1 - u_{i,j}^k)) \tag{10}$$

$$v_{i,j}^{k+1} = v_{i,j}^k + \delta t * (D_v * \left(\frac{v_{i+1,j}^k + v_{i-1,j}^k + v_{i,j+1}^k + v_{i,j-1}^k - 4v_{i,j}^k}{\delta x^2}\right) + u_{i,j}^k {v_{i,j}^k}^2 - (f+k)v_{i,j}^k) \tag{11}$$

III. Method

THIS section will describe the implementation of both the diffusion method and the Monte Carlo method and how they might be compared with each other. It also explains the method used to try to optimise ω for the SOR iterations. Lastly, implementation of the Gray-Scott model will be described.

A. Diffusion method

The diffusion method of DLA requires the solving of the time-independent diffusion equation every single iteration. It is a hefty computation to repeatedly do this from scratch. Since the cluster only adds one lattice point in an iteration, the effect on the diffusion field is quite small. This means that the SOR method can use fewer iterations when starting from the previous diffusion field instead of from scratch - as it should still converge to the same solution. This report uses a stopping condition $\epsilon = 10^{-3}$. Before the very first iteration, the cluster has not grown yet and the environment is "empty". The analytical solution for this situation is known, so the diffusion field is initialised using Equation 4.

1) Optimising ω: The convergence rate of SOR depends on the chosen ω. The optimal ω should have the fastest convergence rate and should thus need the fewest iterations to find a solution (when $\delta < \epsilon$). Golden section search [1, p. 269] is used to find this optimal ω.

However since the DLA diffusion method is stochastic, ω will depend on the random growth of the cluster. To try to combat this, multiple runs are needed to find the average optimal ω. ω is held constant through out a run.

B. Monte Carlo method

The Monte Carlo method is tested with the same initial- and boundary conditions as the diffusion method. Thus the structure starts with a single cell at the centre bottom row of the grid. The grid has periodic bounds in the x-direction.

Random walkers are released from above the structure to simulate the diffusion of the concentration field. There is no need to release the random walker from the top of the grid, since the random walker moves completely randomly and because of the periodic boundary conditions in the x-direction. Instead, the random walker is released from a random position one row above the current height of the structure. This reduces the number of steps a random walker needs to do before it neighbours the structure.

The random walkers are released one at a time. This repeats until the structure has reached the top of the grid.

C. Comparing DLA methods

The diffusion and random walker method are compared with each other through the density of the structures. The density of the structure is given by

$$\rho = \frac{N_{structure}}{N^2}, \tag{12}$$

where $N_{structure}$ is the number of cells which belong to the structure and N is the size of the grid.

With this metric the impact of η on the diffusion method and p_s on the random walker method is quantitatively measured.

D. Gray-Scott model

The Gray-Scott model that is investigated in this report divides the environment into a 100×100 lattice, and uses periodic boundary conditions in both the x- and y-directions, meaning that $u^k_{0,j} = u^k_{N,j}$, $u^k_{i,0} = u^k_{i,N}$, $v^k_{0,j} = v^k_{N,j}$ and $v^k_{i,0} = v^k_{i,N}$. Initially at $t = 0$, the concentrations are initialised at $u = 0.5$ everywhere, $v = 0.25$ in a small square in the centre of the environment, and $v = 0$ everywhere else. This square has sides of length 10, so 10% of the size of the environment sides.

The behaviour of noise is also investigated. This noise is implemented by adding a randomly generated number to each of the initial concentrations at each lattice site (at $t = 0$). This randomly generated number is sampled from a normal distribution with a mean of 0 and a variable standard deviation. The concentration is then capped between 0 and 1, so that it is still a valid value.

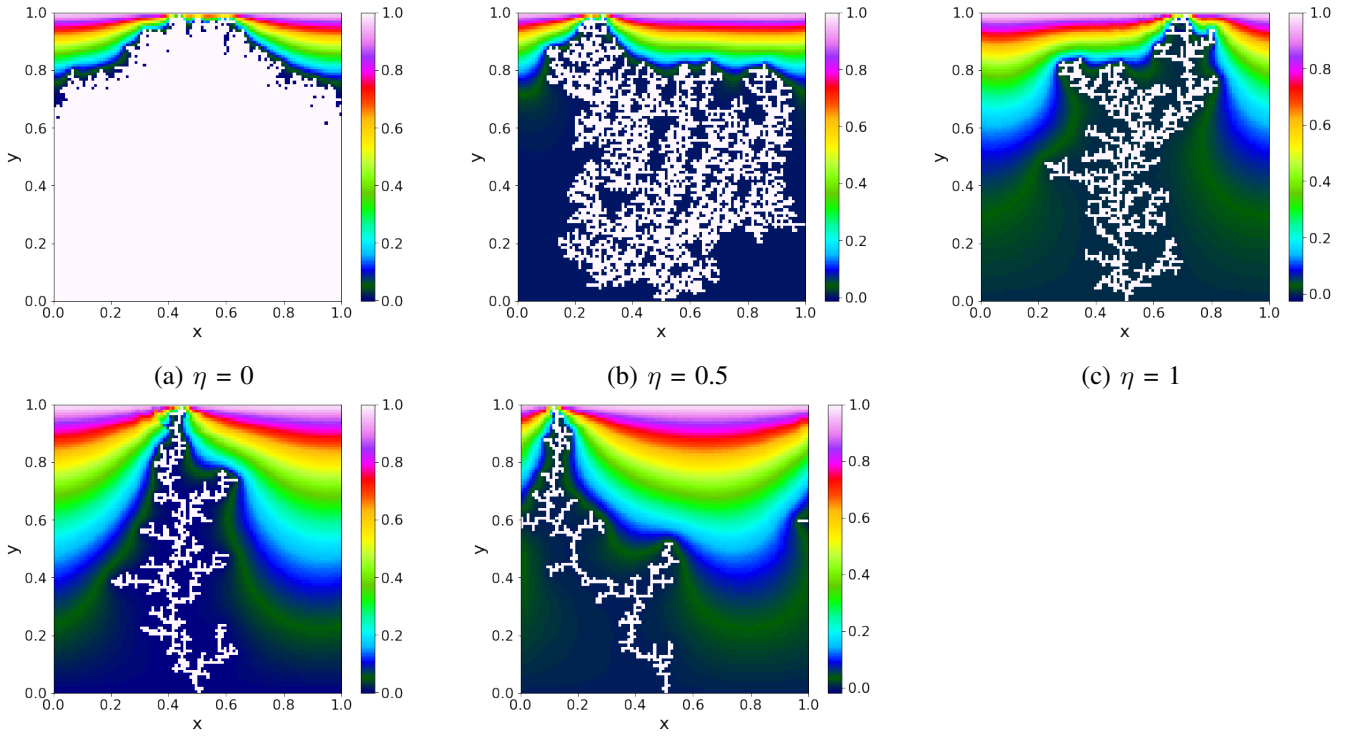
IV. Results

THE results are shown for both the diffusion method and the Monte Carlo method. Example plots of the final state of the cluster for both methods are shown. Also the impact of η and p_s on the cluster density is shown. At last the Gray-Scott model will be shown for different parameters.

A. Diffusion method

The diffusion method is tested for different η values. Figure 1 shows the final state of the cluster, when it first reaches the top. At $\eta = 0$ the Eden cluster is obtained. As η increases the cluster becomes less compact and starts to grow more in a straight line to the top.

The impact of η on the cluster density is shown in Figure 2. The cluster density is largest at low values of η. As η increases, the structure density decreases. This can also visually be seen from Figure 1.



(a) $\eta = 0$ (b) $\eta = 0.5$ (c) $\eta = 1$

(d) $\eta = 1.5$ (e) $\eta = 2$

Fig. 1: Cluster forming for different η values. The grid had a size of 100. The colours show the concentration of the field. The white pixels are part of the cluster. A constant stopping condition was used for the SOR algorithm of $\epsilon = 10^{-3}$, with $\omega = 1.3$.

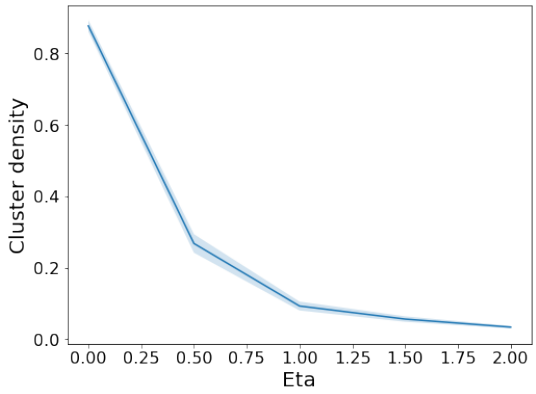


Fig. 2: The structure density as a function of η for the diffusion method. Each run was repeated 10 times. The shaded region shows the 95% confidence interval.

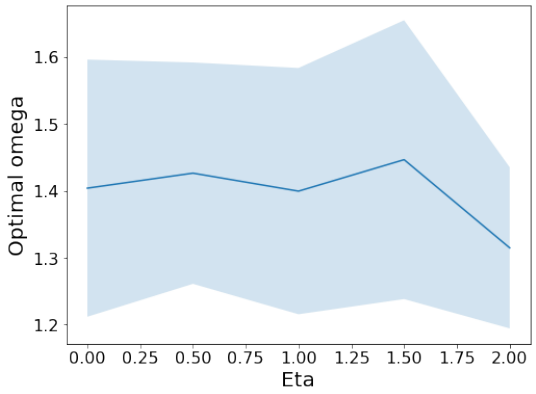
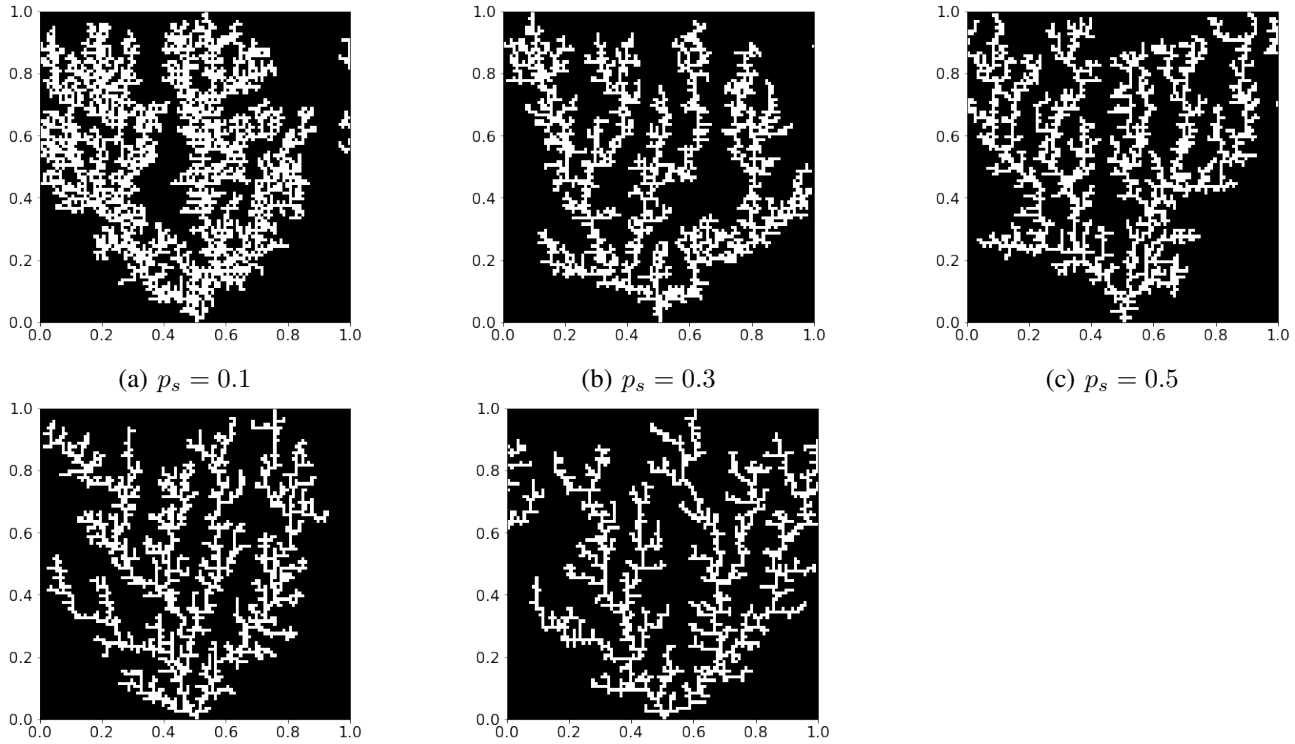


Fig. 3: The optimal ω as a function of η. ω was optimised with Golden Section search. Golden Section search is unable to find a specific optimal ω due to the stochastic behaviour of the system. The optimal ω calculation is repeated 10 times. The shaded region shows the 95% confidence interval.

An attempt was made to optimise ω for the diffusion. The optimal ω for different η values is shown in Figure 3. Each ω optimisation is repeated 10 times. The large confidence interval shows that the optimal ω changes per run. Thus there is no definite best optimal ω. There however does seem to be an average best optimal ω of ~ 1.4, which seems irrespective of η.

B. Monte Carlo method

The Monte Carlo method is tested for different p_s values. Figure 4 shows the final state of the cluster. At low sticking probabilities the cluster is more dense



(a) $p_s = 0.1$ (b) $p_s = 0.3$ (c) $p_s = 0.5$

(d) $p_s = 0.7$ (e) $p_s = 0.9$

Fig. 4: Cluster forming for different values of p_s calculated with the Monte Carlo method. The grid had a size of 100.

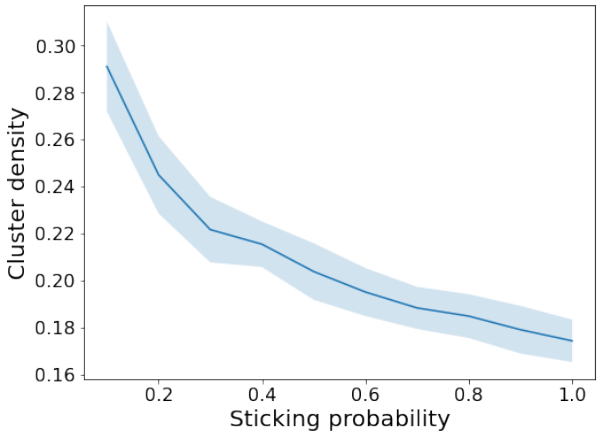


Fig. 5: The structure density as a function of p_s for the Monte Carlo method. Each run was repeated 10 times. The shaded region shows the 95% confidence interval.

compared to higher sticking probabilities.

The impact of the sticking probability on the cluster density is shown in Figure 5. The cluster density is largest at a low sticking probability. As the sticking probability increases, the structure density decreases. This can also visually be seen from Figure 4.

C. DLA method comparisons

The DLA methods can be compared with each other through the cluster density. The sticking probability p_s tries to mimic the η value from the diffusion method. When p_s is set to 1, then this should represent the diffusion method for $\eta = 1$. However the same behaviour is not observed. When $p_s = 1$ then the cluster density is 0.179 ± 0.010. The diffusion method however finds a cluster density of 0.107 ± 0.014. Thus the two methods can not directly be compared without varying the sticking probability.

The Monte Carlo method also has a much more limited range of cluster densities compared to the diffusion method. From Figure 5 it can be seen that the cluster density only ranges from ~ 0.16 to ~ 0.3 for the Monte Carlo method, while the diffusion method ranges from ~ 0.05 to ~ 0.9. Thus only at cluster densities of ~ 0.16 to ~ 0.3 are the methods comparable.

D. Gray-Scott model

The Gray-Scott model investigated in this report uses a 100×100 lattice and default parameter values of $\delta t = 1, \delta x = 1, D_u = 0.16, D_v = 0.08, f = 0.035, k = 0.06, \sigma_{\text{noise}} = 0$. Figures 6-9 show how the behaviour

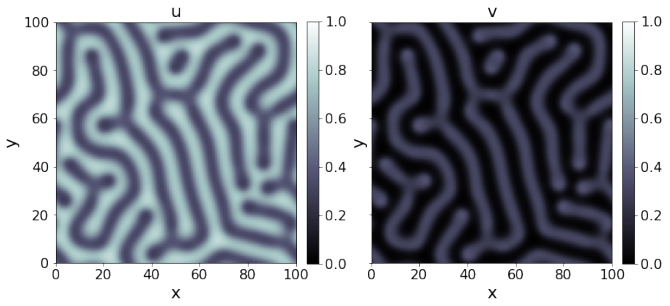


Fig. 6: The simulation of the Gray-Scott model with noise at $T = 10000$ for parameters $\delta t = 1, \delta x = 1, D_u = 0.16, D_v = 0.08, f = 0.035, k = 0.06, \sigma_{\text{noise}} = 0.1$.

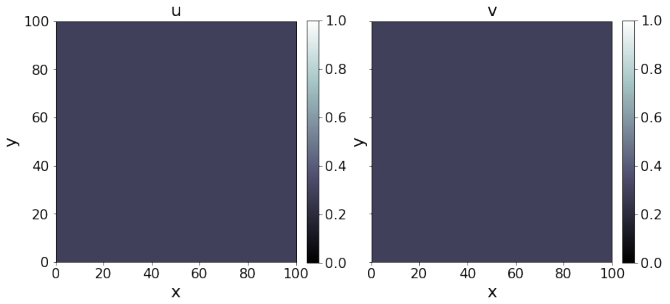


Fig. 7: The simulation of the Gray-Scott model with deviated k at $T = 10000$ with parameters $\delta t = 1, \delta x = 1, D_u = 0.16, D_v = 0.08, f = 0.035, k = 0.05, \sigma_{\text{noise}} = 0.1$.

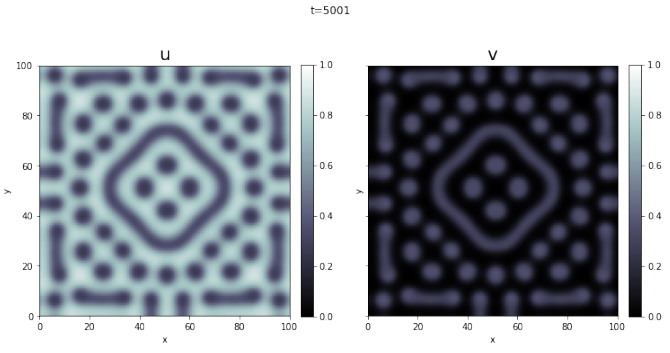


Fig. 8: The simulation of the Gray-Scott model with deviated f at $T = 10000$ with parameters $\delta t = 1, \delta x = 1, D_u = 0.16, D_v = 0.08, f = 0.03, k = 0.06, \sigma_{\text{noise}} = 0.1$.

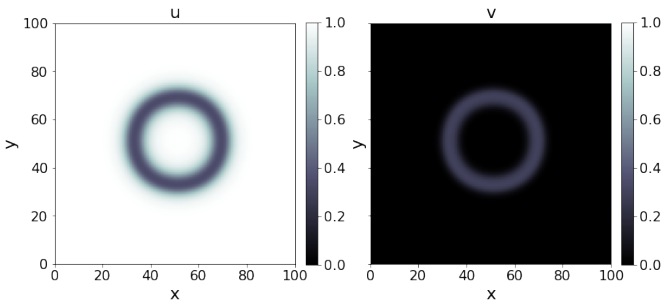


Fig. 9: The simulation of the Gray-Scott model with deviated D_v at $T = 5000$ with parameters $\delta t = 1, \delta x = 1, D_u = 0.16, D_v = 0.1, f = 0.035, k = 0.06, \sigma_{\text{noise}} = 0.1$.

changes when making changes to specific parameters, and these results will be discussed in this section.

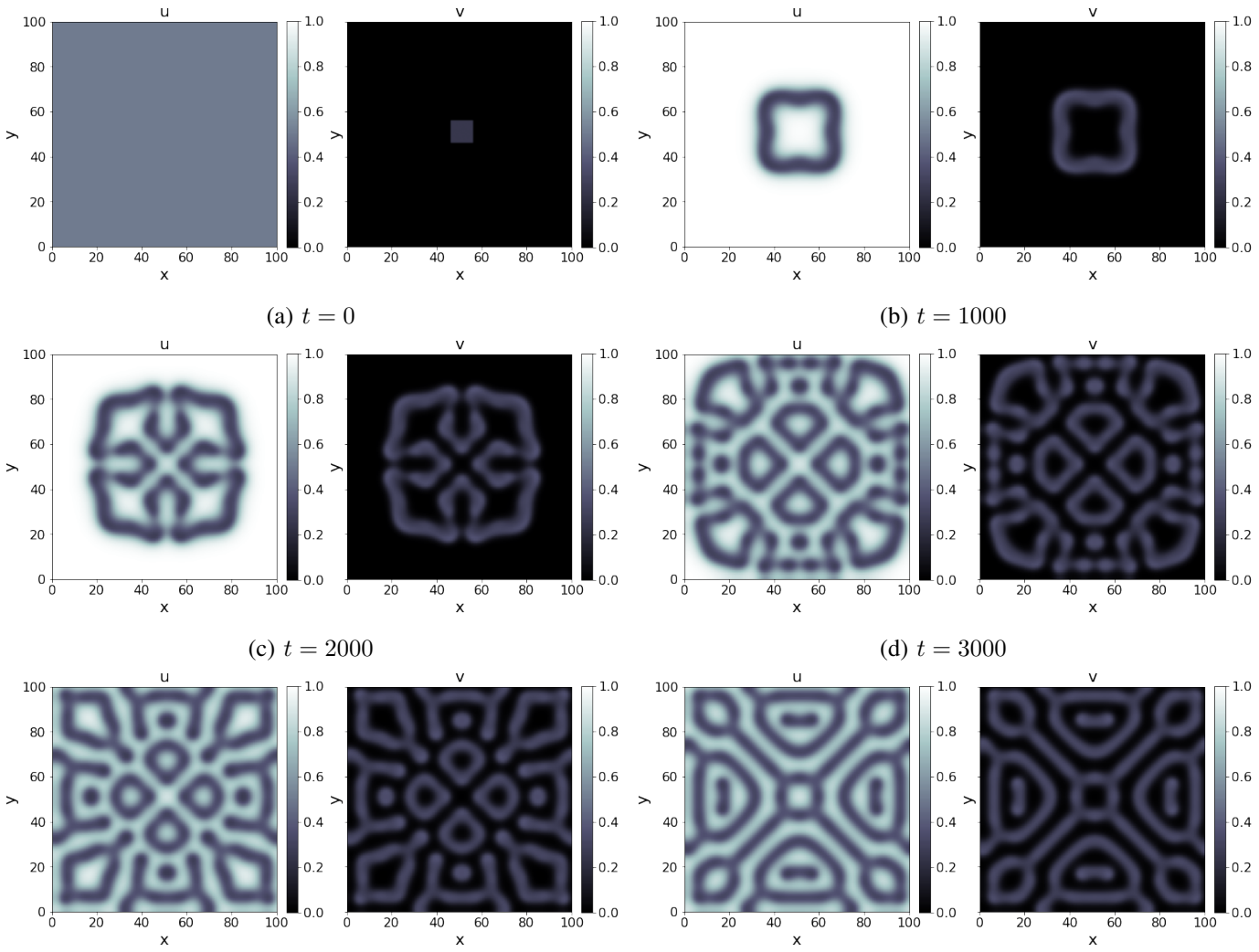
Figure 10 shows the behaviour of the Gray-Scott model through several points in time, using the default parameter settings. Figure 10a shows the concentrations at $t = 0$ - these initial settings are used for all Gray-Scott simulations in this report. First, the small square grows into a rounder shape outline, and then develops into more complex patterns. Because of the periodic boundary conditions and the single centred initial square, the resulting plots are all symmetrical in both the x- and y-direction.

Figure 6 shows how the stable state changes when a small amount of noise is added ($\sigma_{\text{noise}} = 0.1$). This result is unrecognisable from the model without noise, whose stable state is shown in Figure 10f. Instead, a random line pattern seems to form. Due to the random nature of the noise, the patterns are no longer symmetrical. While the resulting patterns are different for every simulation when random noise is present, the same type of line structure emerges every time.

Figure 7 shows the stable state of the model when k is lowered slightly from 0.06 to 0.05. When k is lower, V decays less quickly, as can be seen from Equation 9. Higher values of v result in a faster decrease in u and an increase in v. The reaction no longer forms a stable edge pattern, but the chemicals diffuse through the system and reach a stable state with a consistent concentration of both chemicals everywhere.

Figure 8 shows the stable state when f is lowered from 0.035 to 0.03. A lower f results in a slower supply of U into the system, as is shown by Equation 8. It seems that the reactions now result in a final pattern where the concentrations of V are less connected, and rather form many small separated circles of high v.

Finally, Figure 9 shows the concentration field when D_v is increased from 0.08 to 0.1. In that case, the chem-



(a) $t = 0$ (b) $t = 1000$

(c) $t = 2000$ (d) $t = 3000$

(e) $t = 5000$ (f) $t = 15000$

Fig. 10: Gray-Scott simulation at different time points, showing the concentration of U on the left and the concentration of V on the right, with parameters $\delta t = 1, \delta x = 1, D_u = 0.16, D_v = 0.08, f = 0.035, k = 0.06, \sigma_{\text{noise}} = 0$.

ical V will diffuse through the environment faster. It seems that this faster diffusion slows down the "spread" of the initial small square containing the concentration $v = 0.25$. Instead, a smooth nearly-circular ring emerges in the middle of the environment.

V. Discussion & Conclusion

THE diffusion method was implemented and was able to show the predicted behaviour. As η increases the cluster density drops. The same can be said about the Monte Carlo method. As p_s increases the cluster density drops. These methods however can not directly be compared with each other. The diffusion method is able to produce clusters with a much wider range in cluster densities, while the Monte Carlo method produces a much more narrow range of cluster densities.

Optimising ω is also not feasible for the SOR of the diffusion method, because of the stochastic behaviour of the system. Furthermore, the cluster grows over time, which would require a different ω for each time step. Future research might look into the relation between an optimal ω and the shape of the cluster. This would allow for faster convergence of the diffusion field.

The Gray-Scott model results in striking patterns, which can differ significantly for even slightly different configurations of parameters. This report did not see a configuration that did not result in a stable pattern after many iterations, although future research could be focused on which configurations can affect stability.

References

[1] M. T. Heath, *Scientific Computing: An Introductory Survey*, 2nd ed. Boston: McGraw-Hill, 2002.