Scientific Computing Exercise Set 2

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I. Introduction

THE development of diffusing particles is a fundamental concept in physics to elucidate and prove events in daily life. In this research, we analyze the formation of clusters from particles under different circumstances, and a reaction process using the Gray-Scott model. The patterns created by the equations for the Gray-Scott model, resemble patterns seen in living creatures.

The aim of this research is to study simulation techniques, as the diffusion-limited aggregation (DLA), Monte Carlo methods, and the Gray-scott model, in order to analyze diffusion systems.

To start with, the growth model is implemented by solving the time independent diffusion equation. Therefore, in this assignment, we build upon our previous report and results of the Successive Over Relaxation (SOR) method. Moreover, we continue on the DLA simulation by implementing a Monte Carlo method with a random walker. Besides that, we investigate a reaction-diffusion system with the Gray-Scott model by implementing a square and also noise to the system.

II. Theory and Methods

In this assignment, we practice with implementing various diffusion systems. In the first part (see section III-A) we implement the formation of an object through diffusion-limited aggregation (DLA) is based on diffusing particles, using the SOR method for diffusion. In the second part (section III-B), we simulate the DLA by releasing random walkers on a grid, and let them walk until they hit the cluster, and then add them to the object. Additionally, in the third part (section III-C), we implement the Gray-Scott model, which describes a system of chemical reactions, involving the two chemicals U and V. Both chemicals diffuse in the system, and also react with each other.

A. Diffusion limited aggregation

In this growth model, the growth is started with a single seed, which is small square object in a single lattice point at the bottom of the computational domain. The DLA can be modeled by solving the time independent diffusion equation:

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

which is the Laplace equation. We assume the boundary conditions given in equation 2, the periodic boundary conditions given in equation 3, the spatial discretization, and a 5-points stencil for the second order derivative.

$$c(x, y = 1; t) = 1 \text{ and } c(x, y = 0; t) = 0 \tag{2}$$

$$c(x = 0, y; t) = c(x = 1, y; t) \tag{3}$$

We consider Successive Over Relaxation (SOR) which applies an over-correction of the new iterate:

$$c_{i,j}^{k+1} = \frac{1}{\omega}(c_{i+1,j}^{k} + c_{i-1,j}^{k+1} + c_{i,j+1}^{k} + c_{i,j-1}^{k+1}) + (1-\omega)c_{i,j}^{k} \tag{4}$$

This iterative method converges only for $0 < \omega < 2$. The optimal ω (that minimizes the number of iterations) for our diffusion problems turns out to be somewhere between $1.7 < \omega < 2$. The exact value depends on the grid size N.

Moreover, we locate growth candidates around the cluster. A growth candidate is basically a lattice site

that is not part of the object, but whose north, east, south, or west neighbor is part of the object. Besides that, we assign a growth probability p_g. This probability for growth at each of the growth candidates is calculated by:

$$p_g(i,j) = \frac{c_{i,j}^n}{\sum_{growthcandidates} c_{i,j}^n}, \tag{5}$$

where the probability is derived as a function of the concentration of diffusing nutrients at that growth location. The parameter η determines the shape of the object, where we get for $\eta = 1$ a normal DLA cluster. For $\eta < 1$ the object becomes more compact (with $\eta = 0$ resulting in the Eden cluster), whereas for $\eta > 1$ the cluster becomes more open (and finally resembles say a lightning flash). Subsequently, the growth candidates are added to the cluster with this probability p_g. After this growth step, the diffusion equation is again solved, and the process is iterated for a large number of growth steps.

B. Monte Carlo simulation of DLA

In this part we simulate the growth of an object with a Monte Carlo simulation, starting with a single seed at the bottom of the grid. 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. The Monte Carlo method releases one random walker at a time in the system. It moves randomly in steps with also the 5-point stencil in the grid. Moreover, we start the walkers on a randomly chosen point on the top boundary in order to use the same boundary conditions as with the SOR (eq. 2). Also, we assume the same periodic boundary conditions (eq. 3). If a walker walks out of the system on the top or bottom boundary it is removed and a new one is created instead.

In the Monte Carlo method, the η parameter is not easily variable for the growth probability p_g, and a sticking probability p_s is introduced. The sticking rue can then be stated in the following way: if the walker enters a cell which is a neighbor of the cluster, it stops there with probability p_s. 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.

C. Gray-Scott model - a Reaction-Diffusion System

We implemented the Gray-Scott model, which describes how a set of chemical reactions evolves trough time. In this case, the reaction involves two chemicals, U and V. Both chemicals diffuse in the system, and also react with each other. Four types of different starting conditions are simulated, the simplest being U with a concentration of 0.5 everywhere in the system, and a square of V with a concentration of 0.25 in the center of the domain. The reaction rate at any point in space, is determined by the local concentrations of U and V. The reactions are:

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

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

U is continuously fed into the system, and reacts with V to produce more V. V spontaneously decays into P, a reaction product which is not interacting with U and V. The first reaction is said to be autocatalytic, since the reaction product V enhances the production of itself. If we let u and v denote the concentrations of U and V, the following equations can be formulated:

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

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

where f controls the rate at which U is supplied, and $f + k$ controls the rate at which V decays. For different values of k and f a large variety of behaviors can be observed. Some result in stable patterns, while others remain time-dependent.

The different starting conditions are also simulated with different values for k and f. The values can be seen in table I, and are the standard conditions according to the assignment, or inspired by Munafo's published data. Each type represents a different pattern of diffusion. Type

gamma shows a wormlike effect in the concentration, whereas theta differs by having few or no die-out events. Pi forms stable localized structures.

Starting conditions	k value	f value
Standard	0.035	0.060
#1: type gamma (γ)	0.022	0.051
#2: type theta (θ)	0.038	0.061
#3: type pi (π)	0.062	0.061

TABLE I: Different parameter values of f and k applied in the Gray-Scott diffusion simulations. The starting condition is either of the standard type or of type γ, θ or π, which in the results on Github is ordered with the corresponding number in this table. Other parameters: $\delta t = 1, \delta x = 1, D_u = 0.16, D_v = 0.08, u = 0.5, v = 0.25$. We have applied these initial conditions to a model with a square of v in the center of the system ('object'), and to two models with noise ('noiseA', and 'noiseB').

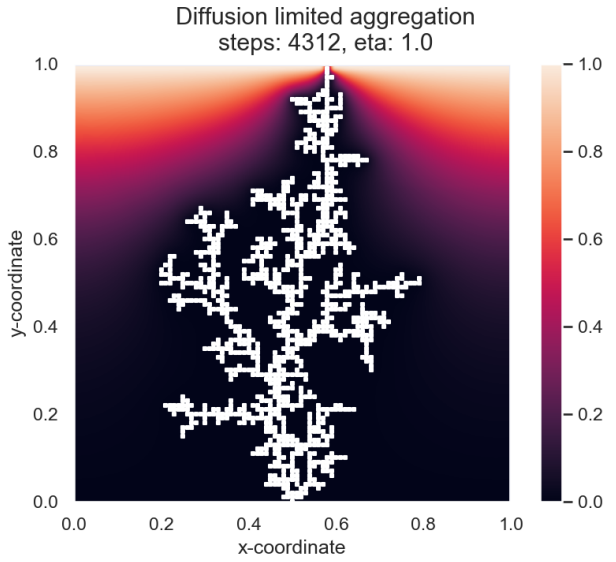

Fig. 1: Simulation of diffusion limited aggregation with the diffusion equation, for $\eta = 1$, with a criterion for convergence of 10^{-2}. The simulation starts with a single seed at the bottom of the computational domain.

III. Results

A. *Diffusion limited aggregation*

The growth model with a grid size of 100x100 was implemented with the SOR method. The simulation is started with a single seed at the bottom of the computational domain and the analytic solution of the diffusion equation. After every addition, we let the diffusion converge for the new object with the SOR method. The result, with an η of 1 is shown in figure 1. The stopping condition for this simulation was to stop if the object reached the boundary of the grid. Moreover, various growth simulations with different growth probabilities p_g (as stated in eq. 5), are shown in figure 3 as a function of η. Here, we simulated until the size of the object was 150 gridpoints, to be able to compare the objects to the ones with the Monte Carlo method. Comparing the plots in figure 3, the object becomes more compact for $\eta < 1$, as shown on the top of figure 3, whereas for $\eta > 1$, the object becomes more open, as illustrated on the bottom of the figure. Considering figure 1, the simulation shows a normal DLA cluster.

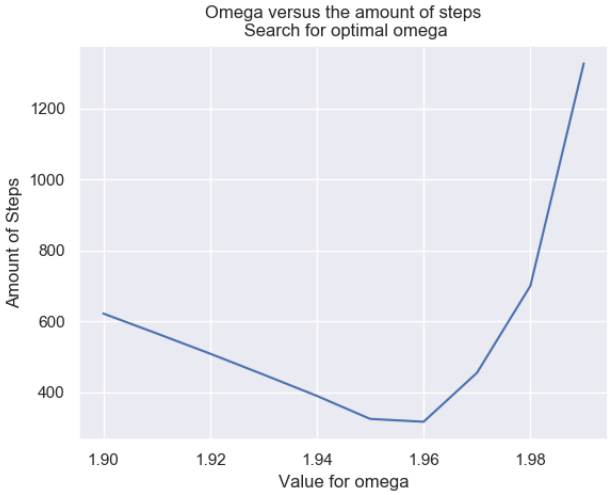

Fig. 2: Shown is a part of the search for the optimal ω for an object of size 25 with an η of 1.0. In fact, the search is done for ω values from 1.7 to 1.99 with steps of 0.001. We see the decline in the amount of steps, and that is very important to pick a suitable ω.

Because our hypothesis was that you can not optimize the omega value for SOR with different shaped objects, we did a search for the optimal omega for different objects and different etas. We did this by trying omegas

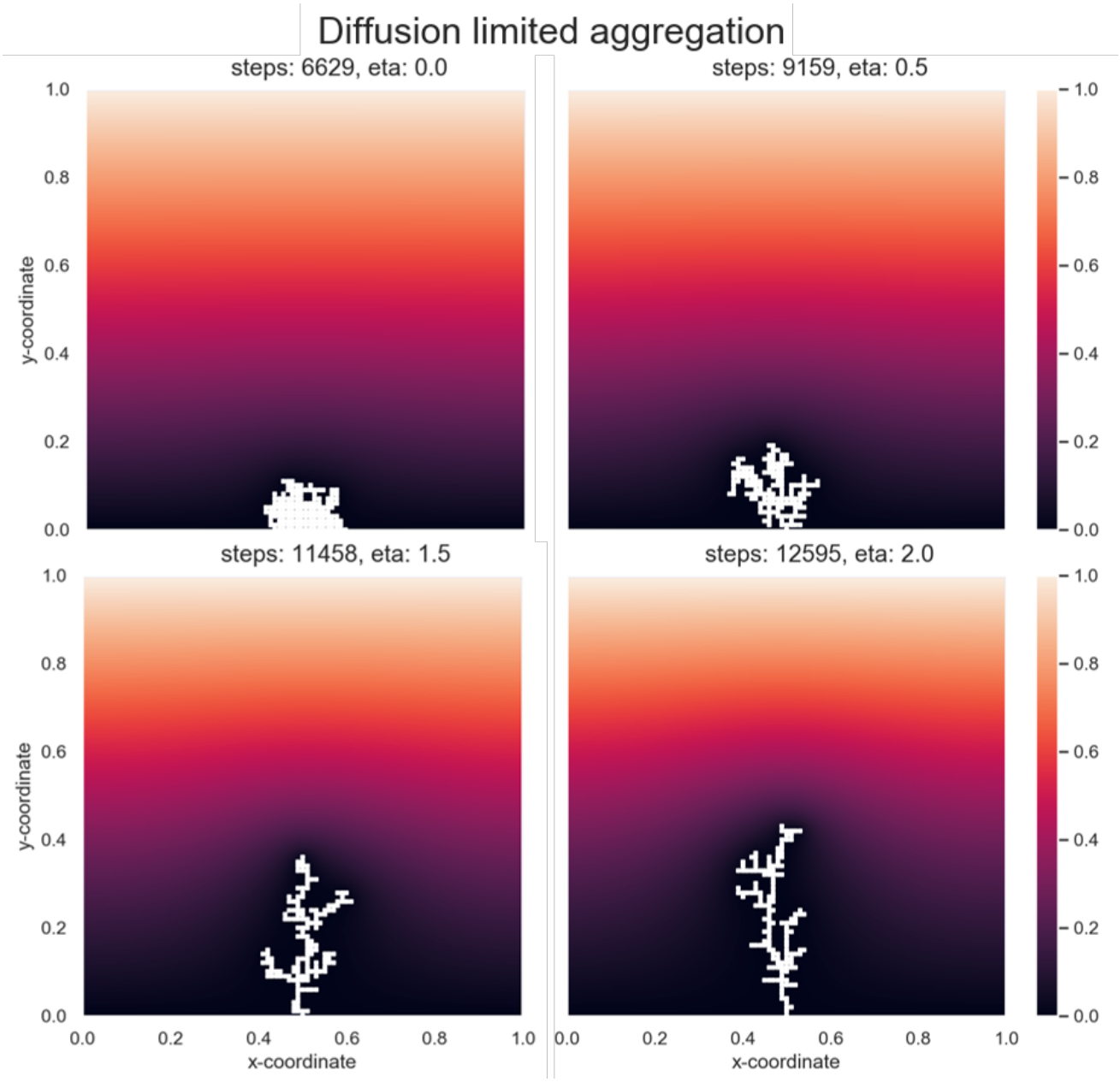

Fig. 3: Simulations of DLA with different values of η. As stopping criterium, a maximum object size of 150 gridpoints is used. The figure shows typical DLA results for different values of η. For $\eta = 0.0$ we receive the Eden cluster and for $\eta = 1.0$ we see the normal DLA cluster. The differences are clear: when η gets smaller, the object that forms becomes more and more compact.

between 1.7-1.99 with steps of 0.01 and calculating the amount of steps for every one of these omegas. The optimal omega is then the one with the least amount of steps. How the optimization works is illustrated in figure 2 for an object of size 25 with an eta of 1.0. We can see that an omega of 1.96 is the best for this case. This is done for different object sizes and different etas. The results are shown in table II: we can see that the omega differs for the different object sizes and etas. The optimal omega also differs a bit between runs with the same η with the same object size, because of the stochasticity of the shape of the object.

		Object Size						
		25	**50**	**75**	**100**	**125**	**150**	**Reached boundaries**
η	**0.0**	x	x	x	x	x	x	1.93
	0.5	1.96	1.96	1.96	1.96	1.96	1.95	1.87
	1.0	1.96	1.96	1.96	1.96	1.95	1.95	1.90
	1.5	x	x	x	x	x	x	1.92
	2.0	x	x	x	x	x	x	1.92

TABLE II: Optimal omegas for different object sizes and different η-s. We can see here that while the object is small, the optimal ω does not differ from the optimal ω calculated in the previous assignment (for a gridsize of 100x100).

B. Monte Carlo simulation of DLA

The diffusion limited aggregation is also implemented with a Monte Carlo model. In the first step, the model contains a single seed for the object at the bottom of the grid, and random walker at a random x location and a y location 5 steps above the seed. The random walker sticks to the object upon arriving at one of the locations next to it. The walker can not walk into the object and when it reaches the upper/lower boundaries it is removed and a new walker is placed. The left/right boundaries are periodic. This Monte Carlo simulation is shown in figure 4. The shape of the object is comparable to the shape of the objects obtained with η-s higher than 1 in the DLA simulation with the diffusion equation.

In the Monte Carlo version of the DLA, the η parameter is not easily variable. Instead, a sticking probability p_s is introduced. Previously in the SOR, the shape of the cluster was dependent on the growth probability p_g which was reliant on the value of η. Therefore, we ran the model with different sticking probabilities. For a simulation with sticking probability 0.1 see figure 5.

The shape of the object ran with a sticking probability of 0.1 is more comparable to the ones with an η of 1.0 or lower. The branches of the objects get thicker. To be able to really compare the heights and widths of the obtained objects with the ones obtained with the diffusion equation we ran the Monte Carlo simulation

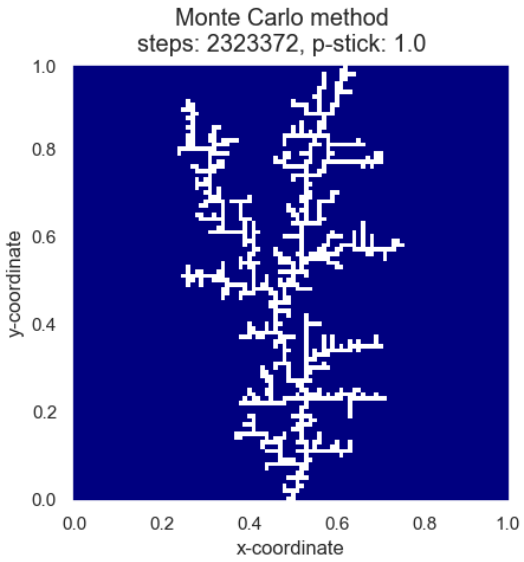

Fig. 4: DLA modeled with a Random Walker with a sticking probability of 1, ended when the growth of the object reaches the upper boundary of the domain.

also until the object reaches a size of 150 gridpoints. We let the random walker start at the top of the computational domain, which took significantly longer then when letting it start a bit higher then the seed. The results are shown in figure 6.

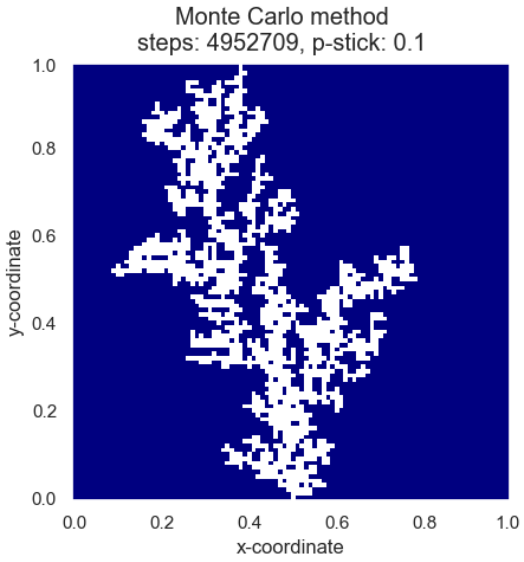

Fig. 5: DLA modeled with a Random Walker with a sticking probability of 0.1, ended when the growth of the object reaches the upper boundary of the domain.

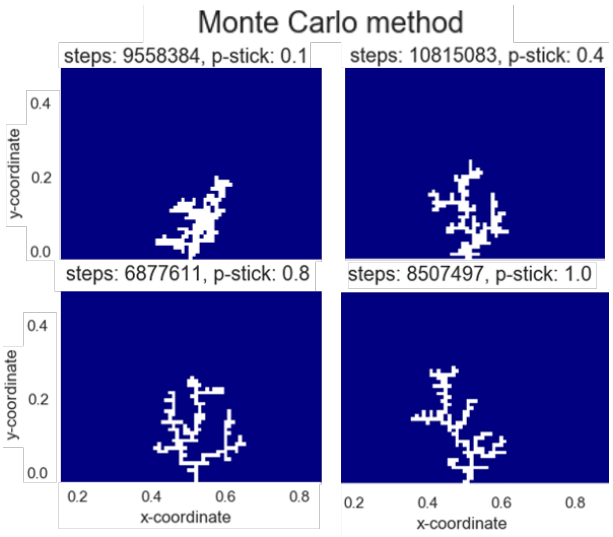

Fig. 6: Diffusion limited aggregation modeled with a Random Walker (Monte Carlo) method with different sticking probabilities. At step 1, a seed of the object is placed at the lowest place in the computational domain. We let the walker do its random walk until the object contains 150 gridpoints.

C. Gray-Scott model - a Reaction-Diffusion System

For the reaction given in equations 6 and 7, the Gray-Scott model is implemented. To implement the model into our program, we discretize equation 8 and 9 to:

$$u_t^{i,j} = u_t^{i,j} + \frac{\delta t D_u}{\delta x^2} \left(u_t^{i+1,j} + u_t^{i-1,j} + u_t^{i,j+1} + u_t^{i,j-1} - 4u_t^{i,j}\right) - u_t^{i,j}(v_t^{i,j})^2 + f(1 - u_t^{i,j})$$

$$v_t^{i,j} = v_t^{i,j} + \frac{\delta t D_v}{\delta x^2} \left(v_t^{i+1,j} + v_t^{i-1,j} + v_t^{i,j+1} + v_t^{i,j-1} - 4v_t^{i,j}\right) + u_t^{i,j}(v_t^{i,j})^2 - (f + k)(v_t^{i,j})$$

for the concentration of U and V, respectively. Besides that, we implemented periodic boundary conditions on each boundary of the domain (i.e. upper/lower and left/right boundaries), as for example mentioned in section II with equation 3 for being periodic in the left/right boundary of the domain.

We simulate the diffusion of both chemicals in the system, while they react with each other. At step 0 in the simulation, the concentration of chemical U is 0.5 everywhere in the system, and the concentration of V is 0.25 in a small block in the center of the computational domain, as shown on the most left plot of figure 7. We see how U spreads trough the system. The reaction diffusion systems are simulated for 5000 steps. For most begin conditions and parameter settings this was enough to reach an equilibrium, which can be seen in figure 8. With different parameter settings (γ), the simulation of object 1 did not end in an equilibrium (see figure 9.

Moreover, the Gray-Scott model with a small amount of noise is shown in figure 10. We can see that the output heavily depends on the initial placements of the reactant V.

	Parameter values			
Starting conditions	**Standard**	**gamma**	**theta**	**pi**
Object 1	stable	unstable	stable	stable
Noise 1	stable	unstable	stable	stable
Noise 2	stable	unstable	stable	stable

TABLE III: The concentration outcomes of the reactants U and V whether they are stable or not within 5000 steps. The results are of Gray-Scott models with a square object ('Object1', and two models with different kind of noise ('Noise 1', and 'Noise 2'). The parameter values are explained in II. Standard: $f = 0.035, k = 0.060$, gamma: $f = 0.022, k = 0.051$, theta: $f = 0.038, k = 0.061$, pi: $f = 0.062, k = 0.061$. Examples are shown in figure 8, and 9.

IV. Discussion

To be able to compare the shapes of the objects of the various DLA simulations better, we should try to express the shape in a number, for example a height/width ratio, and the amount of neighboring object points a point in the object has on average. This way, we could say more easily what η and what P_{stick} are comparable with each other. For a lower sticking probability, the object

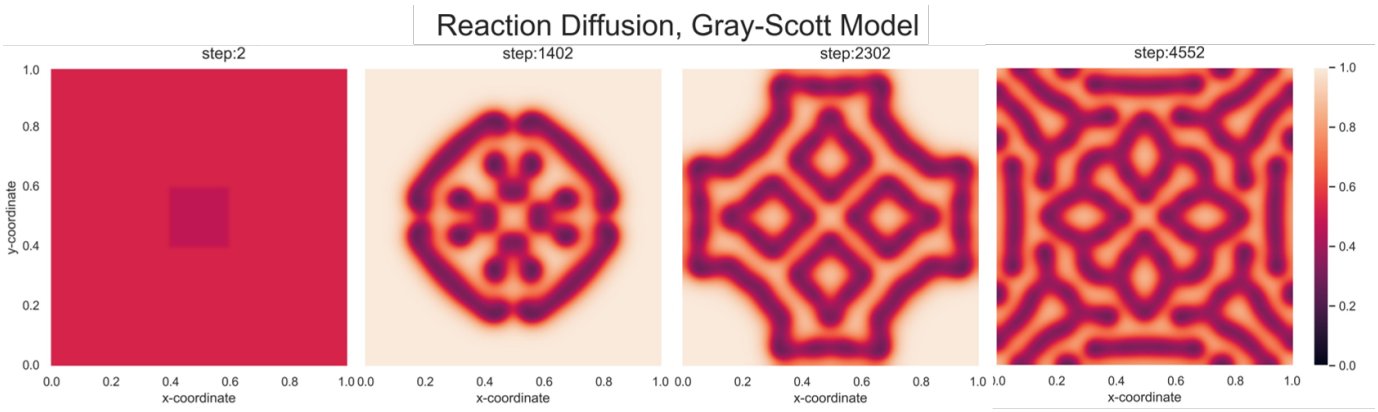

Fig. 7: The diffusion of the reactant u in the reaction-diffusion system as described, modelled with the Gray-Scott model. Parameter values $D_v = 0.08, D_u = 0.16, f = 0.035, k = 0.060$.

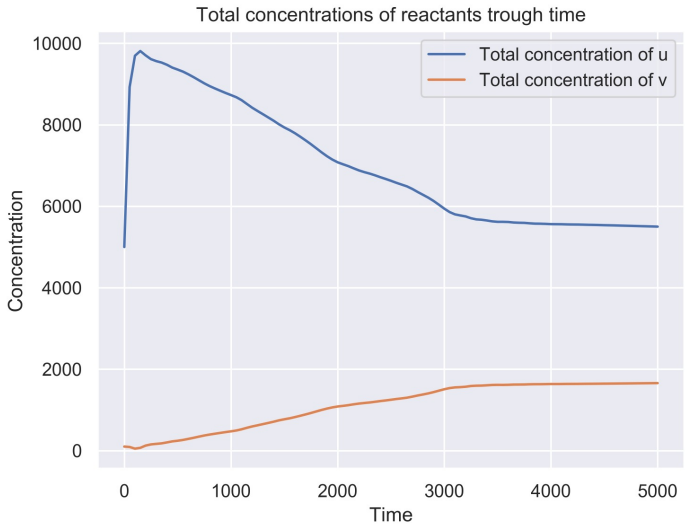

Fig. 8: Concentrations of the reactants U and V through time for the normal object with the standard parameter settings. With these settings, the system reaches an equilibrium after 3500 steps.

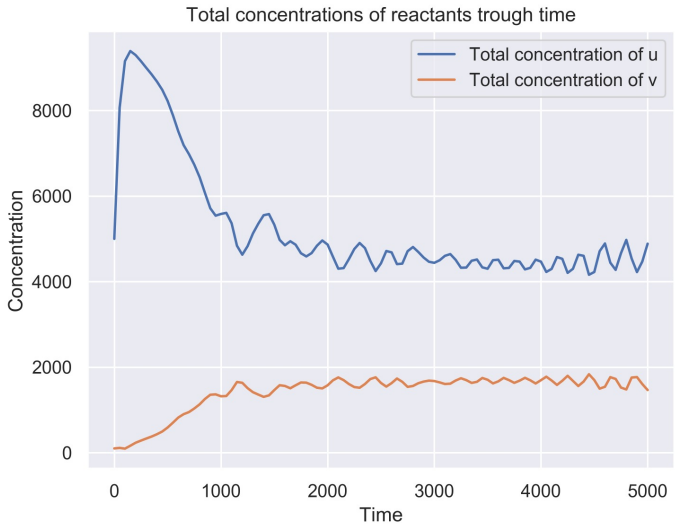

Fig. 9: Concentrations of the reactants U and V through time for the normal object with parameter settings theta. With these parameter settings, the system does not go into equilibrium after 5000 steps.

seems to resemble more like the objects with lower η parameters, but we seem to not reach the Eden Cluster with a sticking probability of 0.1. Of course we could try to lower the sticking probability even more, but this would also slow down the simulation more.

To reduce the time to do the calculations, we could still invest into getting Numba's JIT compiler to work for our code. Also we could have done the optional part of question A to work with our GPU's or with the Google Collaboration community. There are many more options to try to reduce the time of the calculations. The convergence criterion for the diffusion equation can maybe be lower than 10^{-5} and still give the same shapes of objects. This should be tested. The random walker could be placed closer to the object instead randomly at the top of the domain, as we did for the first two pictures, and then it could be tested whether this also gives the same results. If that is the case, it can lower the amount

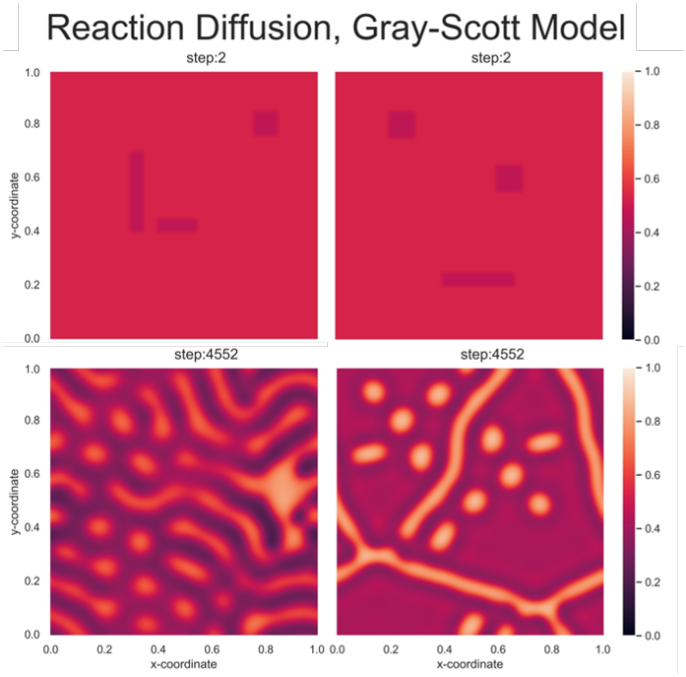

Fig. 10: The diffusion of the reactant U in the reaction-diffusion system as described, modelled with the Gray-Scott model. Left top: starting concentrations Noise 1. Right top: starting conditions Noise 2. Left bottom: End concentrations Noise 1, with parameters type γ: $k = 0.022, f = 0.051$. Right bottom: End concentrations Noise 2, with parameters type π, $k = 0.062, f = 0.061$.

of steps the walker has to take by millions.

When looking at the results for the optimal omega for the SOR convergence, we can also conclude that we can not give the omega a single best value. Nevertheless, we see that the optimal value goes down as the object size increases. Thus, we could calculate the average best omega for example every 100 steps and then change it during the run.

Moreover, the Monte Carlo simulation with a random walker with a sticking probability of 1 has the same shape of the object obtained with η higher than 1 in the DLA. This is because the random walker provides also an more open object when walking through the grid.

Besides that, we analyzed the sticking probability of the random walker. As explained in the results, this probability has the same effect as η in the growth probability of the DLA, as it changes the shape of the object. For a low sticking probability (e.g. 0.1), the branches of the object becomes thicker, because the random walker keeps searching the object while staying around the same spot to stick. To get the real Eden cluster, we should try to lower the sticking probability even more, but we are not sure if we can reach this shape with the random walker. Furthermore, a higher chance of sticking and a higher η (e.g. $p_s = 0.9$ (MC) or $\eta > 1$(DLA)) creates a 'slim' object with a few branches. With a sticking probability of 1, the shape of the object from the Monte Carlo method resembles an η of 1. We do not think we can produce an object that is as high as the object for higher η-s with the Monte Carlo method.

For the Gray-Scott simulations we saw various outcomes. Where the concentration of V starts is a very important factor for the output: the shape of the concentration profile. We see that most parameter values lead to an equilibrium as end state, but when playing with the values, we see that the gamma values for the parameters lead to an unstable end state. To see if these simulations are really unstable or just take longer to converge, they should be simulated longer. For future research, other boundary conditions could be taken into consideration. Also, the influence of the other parameters, D_v, D_u, dx and dt could be investigated.

V. References

We would like to refer to the assignments of this years course Scientific Computing at the UvA in Amsterdam, and the lecture slides for most of the theory. For the Gray-Scott model we also refer to the website with published data from Robert Munafo, where we got the inspiration for our parameter choices: http://mrob.com/pub/comp/xmorphia/index.html.