THE GRAY-SCOTT SYSTEM ON A GROWING DOMAIN YIELDS FRACTAL-LIKE PATTERNS

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Abstract. Fractal-like patterns were obtained by computer simulations of Gray-Scott equations on a grid that periodically doubles in size. Sample images are presented along with a detailed description of the method to produce them. The standard Gray-Scott parameters, f and k, and the time between doublings were varied systematically to investigate a range of possibilities.

1. Introduction. Reaction-diffusion equations were shown by Alan Turing [12] to describe how relatively simple chemical systems could give rise to various patterns (Turing patterns) often seen in nature. A common example is a leopard's spots. It is tempting to think that to genetically encode spots, information about number of spots and locations of each spot would be needed. Instead, a system of a few interacting chemicals is all that is needed to get regularly spaced spots distributed over the leopard's body.

In this paper we will explore a specific example of the reaction-diffusion equation, the Gray-Scott system [4]. We will see how this system of two equations with two reactive components can create various patterns. Afterward, multi-scaled reaction-diffusion systems [8, 9] will be discussed and the Gray-Scott system will be extended into multi-scale behavior through grid doubling.

1.1. Single-scale reaction-diffusion systems. Let's begin by introducing the general reaction-diffusion equation,

$$\frac{\partial \vec{c}}{\partial t} = \boldsymbol{D}\nabla^2\vec{c} + \vec{R}(\vec{c}),$$

where $\vec{c}$ is a set of concentrations of chemicals, t is time, $\boldsymbol{D}$ is a set of diffusivities, ∇^2 is the Laplace operator, and $\vec{R}$ is a set of reaction functions that can each depend on any subset of concentrations.

The first term, $\boldsymbol{D}\nabla^2\vec{c}$, is called the diffusion term. Basically, the diffusion term will blur nearby concentrations together. Some substances blur more rapidly, so they would have a larger diffusivity (a higher value in the set of diffusivites, $\boldsymbol{D}$).

The second term, $\vec{R}(\vec{c})$, is the set of reaction functions. These tend to model chemical kinetics through collision theory. In many studied versions of the reaction-diffusion equation [1, 3, 4], these reaction functions are nonlinear (a common feature of chaotic systems [11]). Most importantly, these reaction functions tend to sharpen (unblur) the differences of nearby concentrations. Thus the diffusion term and the reaction functions tend oppose each other.

A simple example of a reaction-diffusion equation is Fisher's equation [3].

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + rc(1-c)$$

In Fisher's equation (not the Fisher equation, that is something else) the concentration varies in one direction, x, and in time, t. This was originally used to discuss how newly evolved advantageous traits take over in a population.

A more complicated example, the system of equations that are used in this paper, is called the Gray-Scott system of equations [4]. There are a few great tutorials available online to get

started: `http://www.karlsims.com/rd.html` and `http://mrob.com/pub/comp/xmorphia/`, but a summary also follows here. Below is the Gray-Scott system of equations:

$$\frac{\partial A}{\partial t} = D_{\mathrm{A}}\nabla^2 A - AB^2 + f(1 - A)$$

$$\frac{\partial B}{\partial t} = D_{\mathrm{B}}\nabla^2 B + AB^2 - (f + k)B$$

In the Gray-Scott system, there are two substances diffusing and reacting. A represents the concentration of substance A, and B represents the concentration of another substance, B. D_{A} is the diffusivity of A. D_{B} is the diffusivity of B. f and k are scalar parameters.

In the Gray-Scott system of equations, there are a couple of reaction terms to consider. At the end of the day, the system is quite complicated, and understanding all of the underlying mechanisms is not essential, but a brief summary of the process this system could be describing is given below.

Two of the reaction terms come from a chemical reaction that would correspond to a collision mechanism of:

$$\mathrm{A} + 2\mathrm{B} \rightarrow 3\mathrm{B}$$

This process is call "auto-catalysis." Basically, when two molecules of B collide with a molecule of A, the A turns into B. This reaction accounts for the $-AB^2$ and the $+AB^2$ in the first and second equations in the system. You might expect a rate constant for these terms, but that parameter has been absorbed into our definition of concentration without loss of generality due to the scalability of nature.

These B atoms die after some time, with a rate constant of $f + k$. Here you might expect a single parameter, but it works out nicer if the rate constant for the death of B is always higher than f, thus we use a compound parameter for this rate constant. Thus, it is an exponential dying off of B that accounts for the $-(f + k)B$ term in the second equation of the system.

The last term we need to account for is the $+f(1 - A)$. This term makes most sense in the original context of the Gray-Scott equations, a bunch of interconnected continuously-stirred reactors. A continuously-stirred reactor is a large tank that is stirred so well that any two samples from it are identical (the stirred fluid is homogeneous). A continuously-stirred reactor usually has an inflow with only reactant. In our case, that inflow has only A at a concentration of 1. Thus, this inflow tends to restore the concentration of A toward 1 and in a manner more extreme the further A is from 1.

Regardless of its underlying mechanisms, this system of equations has some neat behavior. We can investigate the behavior by setting up a computer simulation. The technique we will use is called the finite-difference method. Just like how a computer discretizes a picture into pixels, we can discretize the equations and the domain the equations act on.

We imagine a sheet of cells aligned on an even two-dimensional grid (Figure 1.1); this is our domain. We can define the distance between two abutting cells as h. Similarly, we can discretize the small jump forward in time. Thus we can switch notation from ∂t to Δt, because the change in time is no longer infinitesimal. The value of Δt will have to be "small" to keep the simulation stable.

Each cell has a concentration of A and a concentration of B. Thus, cell 1,1 would have associated $A_{1,1}$ and $B_{1,1}$. The changes in concentrations over discrete amounts of time will also be discrete,

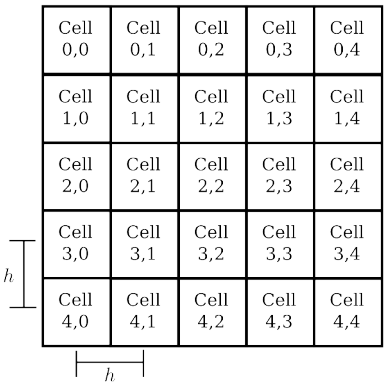

FIG. 1.1. *The reaction area is split into equally sized cells*

so we can also adopt the Δ notation for the concentrations. Thus, the left sides of the equations can be written as:

$$\frac{\Delta A}{\Delta t} = ...$$

or

$$\frac{\Delta B}{\Delta t} = ...$$

The right sides (for now represented as ...) are a bit trickier to determine. Actually, it is only the Laplace operator that is tricky; the other terms only consider the local concentration for a given cell. But we still need to discretize the Laplace operator. Remember, the idea of the Laplace operator is to compare the concentration in one cell to the concentrations in its surrounding cells. It might be tempting to only look above, below, left, and right, but because we have discretized the domain, we really should also consider the diagonals. It has been shown [6] that for large curvatures, the stencil that is most symmetric to rotation is:

$$\begin{bmatrix} 0.05 & 0.20 & 0.05 \\ 0.20 & -1.0 & 0.20 \\ 0.05 & 0.20 & 0.05 \end{bmatrix}.$$

Thus, at cell 2,3 we would say that:

$$\nabla^2 A_{2,3} \approx \frac{0.05A_{1,2} + 0.20A_{1,3} + 0.05A_{1,4} + 0.20A_{2,2} - 1.0A_{2,3} + 0.20A_{2,4} + ...}{h^2}$$

We need a new symbol for this discrete version of the Laplace operator. The conventional choice would be a bold uppercase D, but we used that for the set of diffusivities, so we will use a diamond.

$$\diamondsuit^2 A_{2,3} = \frac{0.05A_{1,2} + 0.20A_{1,3} + 0.05A_{1,4} + 0.20A_{2,2} - 1.0A_{2,3} + 0.20A_{2,4} + ...}{h^2}$$

Now we can write the discretized form of the Gray-Scott system of equations for a given cell (Cell i, j).

$$\frac{\Delta A_{ij}}{\Delta t} = D_A \diamondsuit^2 A_{ij} - A_{ij}B_{ij}^2 + f(1 - A_{ij})$$

$$\frac{\Delta B_{ij}}{\Delta t} = D_B \diamondsuit^2 B_{ij} + A_{ij} B_{ij}^2 - (f+k) B_{ij}$$

or

$$A_{ij}|_{t+\Delta t} = A_{ij}|_t + \Delta t \left(D_\mathrm{A} \diamondsuit^2 A_{ij} - A_{ij} B_{ij}^2 + f(1 - A_{ij}) \right)$$

$$B_{ij}|_{t+\Delta t} = B_{ij}|_t + \Delta t \left(D_\mathrm{B} \diamondsuit^2 B_{ij} + A_{ij} B_{ij}^2 - (f+k) B_{ij} \right),$$

where the | is read as, "at." So $A_{ij}|_{t+\Delta t}$ is the concentration of A in cell i, j at time $t + \Delta t$. You might laugh and say, "That looks almost exactly like what we had two pages ago!" I would have to concede, but we did at least define $\diamondsuit^2$.

One matter we did not discuss is what to do at the edges of our domain. We will use periodic boundaries, like those in Pac-Man or on a torus, such that if we are determining the discrete Laplacian of the concentration in a cell on the right border, like $\diamondsuit^2 A_{2,4}$ from Figure 1.1, we will sample from the left border, like from $A_{1,0}$, $A_{2,0}$, and $A_{3,0}$, as part of the summation.

We have not discussed the initial conditions. There is some flexibility in this, but for now we will start all but one of the cells with A at 1 and B at 0. The special cell will start with A at 0 and B at 1. We might as well put that special cell in the middle.

For an example, we can set:

$$\begin{aligned} f &= 0.057 \\ k &= 0.062 \\ D_A &= 1.0 \\ D_B &= 0.5 \\ h &= 1.0 \\ \Delta t &= 0.5 \end{aligned}$$

The simple 5 by 5 grid would evolve as:

$$A|_{t=0} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \quad A|_{t=0.5} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 0.975 & 0.9 & 0.975 & 1 \\ 1 & 0.9 & 0.528 & 0.9 & 1 \\ 1 & 0.975 & 0.9 & 0.975 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

If this simulation is done on a larger grid and a couple random points are selected as the special starting points, we can get a movie, which is represented in Figure 1.2 by a series of stills. The resulting pattern is reminiscent of brain coral.

A lot of the values of the parameters should have seemed a bit arbitrary. By altering the values, many other patterns can be obtained. In particular, changing f and k can give some interesting variation. In Figure 1.3, a similar simulation to that run in Figure 1.2 is run, but with f and k varying over the domain (grid). We see that for most pairs of f and k, one substance will dominate the other. However, there are some interesting patterns in between the extremes. As we traverse from left to right, we see all black, white dots, striped, black dots, and all white.

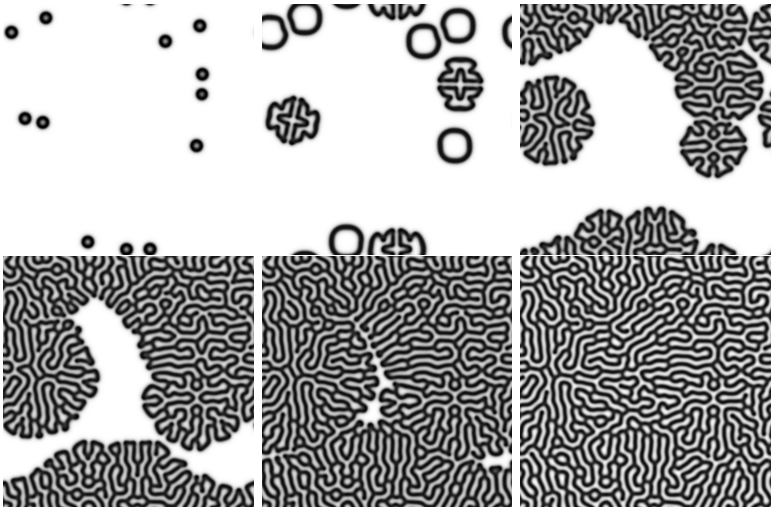

FIG. 1.2. *The spots of B (black) grow to fill the space with regularly spaced, but irregularly patterned, stripes*

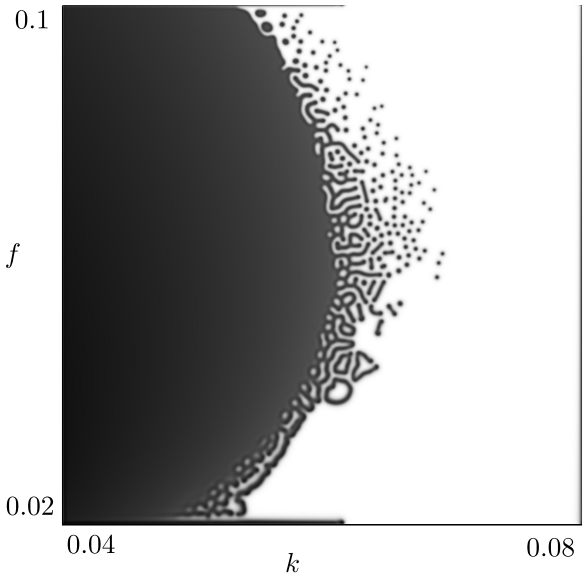

FIG. 1.3. *For most pairs of f and k the domain becomes overrun by A (white) or B (black). There is an interesting region around $k = 0.6$ where white dots on black, stripes, or black dots on white appear.*

One recent finding that adds evidence for reaction-diffusion equations actually having a role in biological patterning comes from fish [9]. Two closely related fish species had different patterning. One had light dots on a dark background, and the other had dark dots on a light background. When these two species were hybridized, the resulting pattern was striped. Thus, in that case too, it seems that stripes are in between light spots and dark spots.

1.2. Multi-scaled reaction-diffusion systems. It has been suggested that some patterns are not satisfactorily explained by single-scaled processes. Before we saw that, for a given set of parameters, we tended to get lines or dots of a certain size. But sometimes biology produces lines inside of dots or dots inside of lines. Research has been done on two-scaled reaction-diffusion systems to investigate those types of patterns inside of patterns [14]. That research inspired a professor of art to create many-scaled Turing patterns with an algorithm inspired by the reaction-diffusion systems [8]. The resulting artwork is stunning and reminiscent of electron microscopy images of diatoms. The many scales give the images a fractal-like quality, in that there are structures of large and small scales. There has also been recent interest in reaction-diffusion patterning on growing domains [2, 5, 7, 10, 13]. It seemed reasonable to expect that a growing domain could provide a context under which a simple Gray-Scott mechanism could provide multiple scales of structure, maybe in a fractal-like manner. The rest of this paper discusses a foray into this realm.

2. Gray-Scott simulations on a growing and pseudo-randomly reseeding domain. In order to get the Gray-Scott system of equations to exhibit multi-scaled behavior, a growing domain is implemented. The grid intermittently doubles in physical size (length) and quadruples in the number of gridpoints (when two-dimensional), such that the new grid has the same spacing between neighbors. The old grid is interpolated to determine the values on the new grid. It is as if each cell has made 3 copies of itself, and the new cells take on concentrations similar to their neighbors.

If we maintain the notation of the first cell having coordinates (0,0) and we call the larger grid of concentrations A^*, then we can say:

$$A^*_{ij} = \begin{cases} A_{\frac{i}{2},\frac{j}{2}} & \text{if } i \text{ and } j \text{ are even} \\ \frac{A_{\frac{i+1}{2},\frac{j}{2}} + A_{\frac{i-1}{2},\frac{j}{2}}}{2} & \text{if } i \text{ is odd and } j \text{ is even} \\ \frac{A_{\frac{i}{2},\frac{j+1}{2}} + A_{\frac{i}{2},\frac{j-1}{2}}}{2} & \text{if } i \text{ is even and } j \text{ is odd} \\ \frac{A_{\frac{i+1}{2},\frac{j+1}{2}} + A_{\frac{i+1}{2},\frac{j-1}{2}} + A_{\frac{i-1}{2},\frac{j+1}{2}} + A_{\frac{i-1}{2},\frac{j-1}{2}}}{4} & \text{if } i \text{ and } j \text{ are odd} \end{cases}$$

Again, we would sample across the periodic boundary at the boundary. Remember, when I say grid doubling, each length doubles, so in two dimensions the number of gridpoints actually increases by a factor of four. So if A was a 5x5 grid, then A^* is a 10x10 grid. We would use an equivalent interpolation scheme for B.

To add some variation, we will also seed new spots of B when we double our grid. Each gridpoint will have an equal chance to seed. Therefore, there will be more simultaneous seeds when the grid becomes large. This will give many small dots and a few big dots. This seeding may seem like a tricky means to get large and small structures, but it is a natural recursion of our initializing a spot at all. If a spot magically appears in the beginning, why shouldn't other spots magically appear later?

An outline of one possible algorithm is:

- Start by making coarse grid (10x10) where everywhere $A = 1$ and $B = 0$
- Loop for 6 rounds:
  1. Give each gridpoint a small chance (0.01) to switch to $A = 0$ and $B = 1$
  2. Make a new larger grid and interpolate concentrations from old smaller grid
  3. Run the finite-difference method of Gray-Scott about $k = 100$ times
- Print the picture

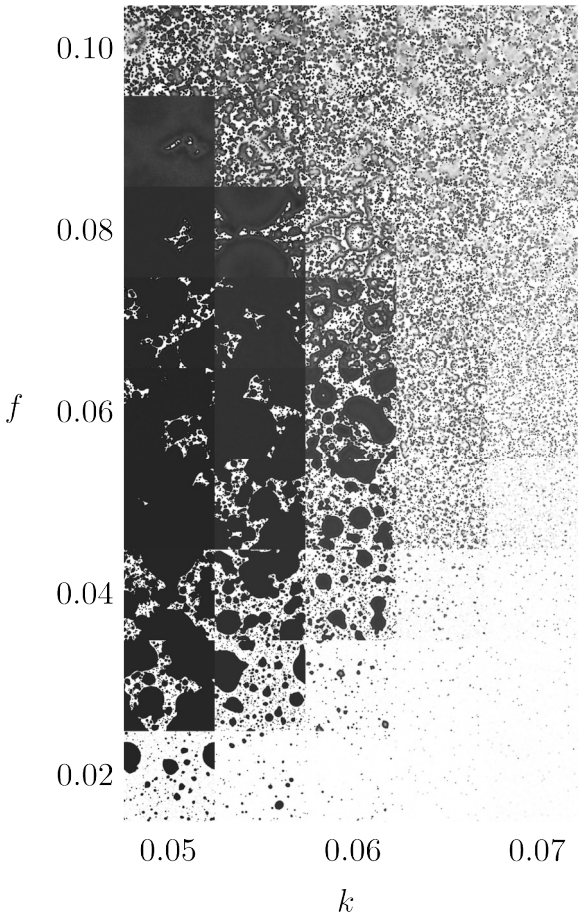

FIG. 2.1. *The described algorithm was run for a variety of pairs of f and k. The results are similar to Figure 1.3; the left side is more filled with black, the white side is more filled with white, and the more interesting behavior is in between.*

This algorithm was run while systematically altering f and k. The results are shown in Figure 2.1

By making minor changes to the described algorithm, some intriguing patterns were formed (Figure 2.2). Some elements altered were the order of operations in the loop, the initial size of the grid, the chance of seeding, the iterations between loops, whether some spots were put down non-randomly, and number of loops. In all of the images shown, D_{A} and D_{B} were left unaltered.

3. Discussion. An algorithm for creating images with multiple scales of structure was presented. Specifically, the algorithm used Gray-Scott system applied to a growing domain. It was shown that a wide variety of results were possible by varying the algorithm and parameters. It was suggested that these types of patterns could manifest in organisms that undergo patterning while growing; however, no strong evidence of this was provided.

These images have aesthetic appeal and are reminiscent of organic forms. Beyond that, the images are fully tileable, so their potential use in UV mapping (texturing 3D models) is exciting.

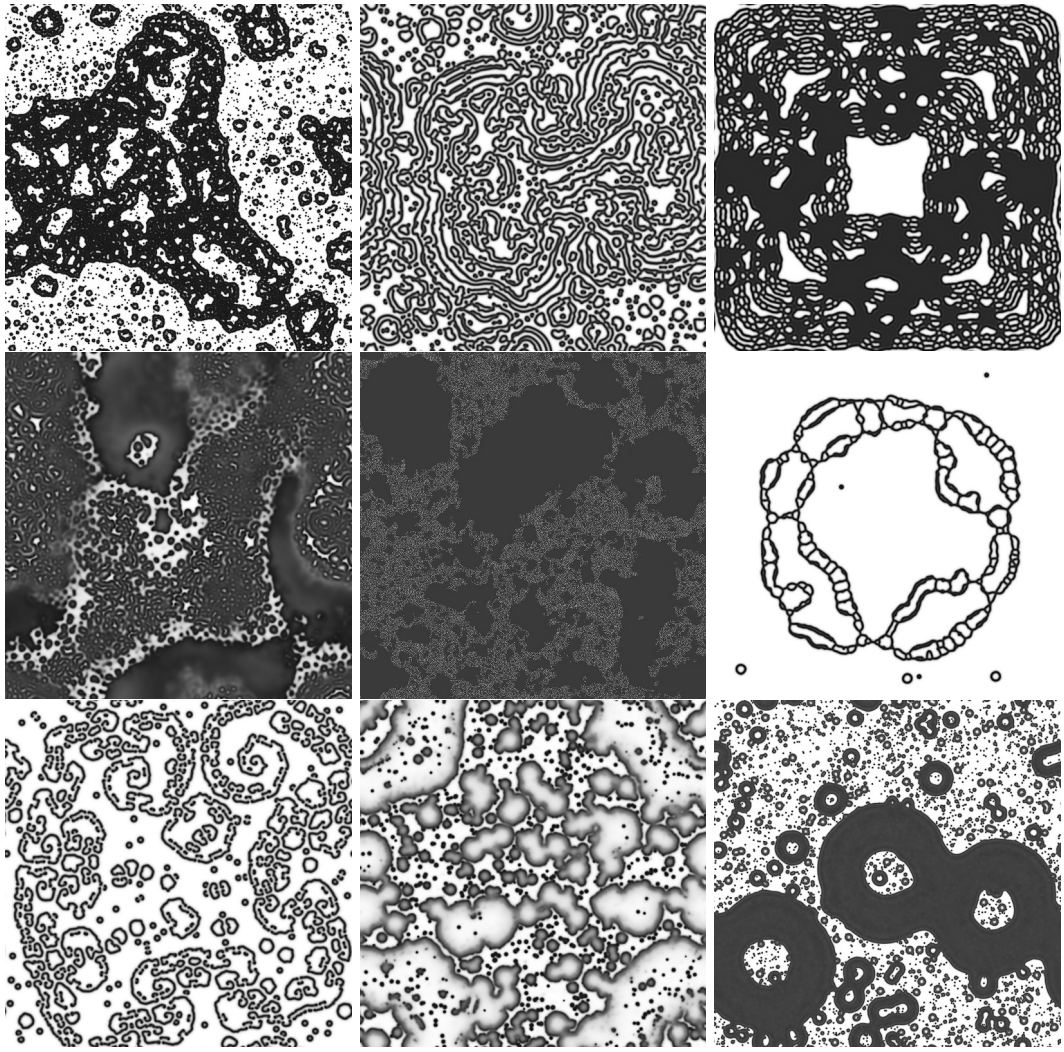

FIG. 2.2. *A wide variety is possible with minimal variations of the algorithm.*

Some of the patterns are also similar to camouflage.

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