PATTERN FORMATION BY REACTION-DIFFUSION

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PROBLEM DEFINITION

In biology, embryological development of the structure of an organism or limb is referred to as *morphogenesis*. As a result of morphogenesis, complex shapes and patterns can form starting from just a single cell. Two main mechanisms that contribute to the embryo's development are *cell movement* and *cell specialization* based on cell position. These mechanisms are influenced by special chemical substances created and released in a cell called *morphogens*. Morphogens freely diffuse from one cell to another through cell membrane and their local concentration at each cell affect the development of that cell.

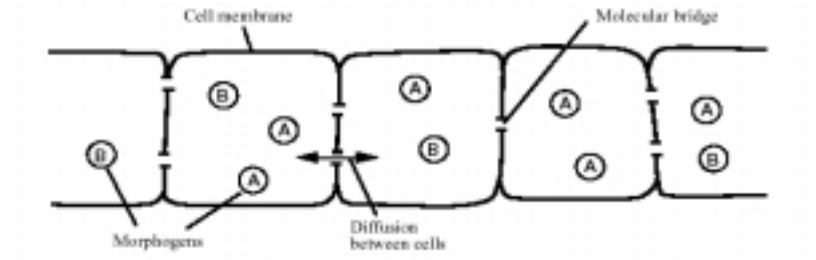

Figure 1. Two morphogens diffusing in a line of cells. [taken from Turk]

The first mathematical model of morphogenesis was proposed by Alan Turing in his 1952 paper "*The Chemical Basis of Morphogenesis*". In his model, there are two morphogens *a* and *b*. They tend to diffuse from higher concentration to lower concentration [Figure 1]. For example, if a particular cell has a higher concentration of chemical b than its neighbors, then that cell's concentration of b will decrease over time by diffusion to its neighbors. Likewise, if the concentration of b is at minimum at a particular place along the row of cells, then more of b will diffuse from adjacent cells to this cell to raise the concentration of b at that cell. Diffusion is not the only mechanism changing the concentration of morphogens; the morphogens can also react with each other. The outcome of the reaction depends on the amount of morphogens a and b already in the cell. In its general form, the changes in concentration of these morphogens over time can be described by the following non-linear partial differential equations:

$$\begin{aligned} \frac{\partial a}{\partial t} &= D_a \nabla^2 a + F(a,b) \\ \frac{\partial b}{\partial t} &= D_b \nabla^2 b + G(a,b) \end{aligned} \tag{1}$$

F(a,b) and G(a,b) are the reaction terms, ∇^2 is the Laplacian operator and D_a and D_b are the diffusion rates for morphogens a and b respectively. This model is known as the *reaction-diffusion* model (RD). Using this model and an initial configuration, one can calculate the concentrations of a and b in a cell at a given time t. However, it is not easy to find closed-form solutions of these equations except when F and G functions are very simple. Therefore, they are discretized and solved numerically. Turing used the following discrete form in one-dimension:

$$\begin{aligned} \Delta a_i &= D_a(a_{i+1} + a_{i-1} - 2a_i) + k(16 - a_i b_i) \\ \Delta b_i &= D_b(b_{i+1} + b_{i-1} - 2b_i) + k(a_i b_i - b_i - 12 - \beta_i) \end{aligned}$$

where a_i and b_i are the concentrations of a and b at i^{th} cell, k is the reaction rate and β_i is the small random substrate in the i^{th} cell. Initial concentrations of both morphogens at each cell are set as 4.0. Without the β_i term, the equations would always evaluate to zero and concentrations would not change over time. Turing found that if diffusion rates are different (i.e. one morphogen diffuse more rapidly than the other) and initial concentrations of morphogens over the cells have random perturbations (as is the case when $\beta_i \neq 0$), a reaction-diffusion system acting over a ring of cells could form a stable pattern of peaks and valleys of chemical concentration [Figure 2]. However, these are not sufficient conditions for convergence, and if parameters in the equations are not care-

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fully selected, the system may show oscillatory behavior, or concentrations of morphogens may increase or decrease unboundedly.

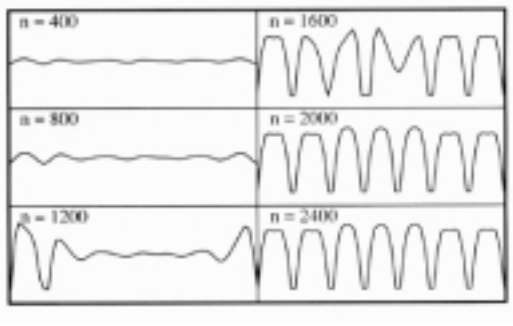


Figure 2. One dimensional example of reaction diffusion. Concentration of b. D_a=0.25, D_b=0.065, k=0.03125, B_i = 0.05 (taken from Turk)

It is possible to extend one dimensional reaction-diffusion model to multiple dimensions. In two-dimensional case, we have the following update equations:

$$\Delta a_{i,j} = D_a(a_{i+1,j} + a_{i-1,j} + a_{i,j+1} + a_{i,j-1} - 4a_{i,j}) + k(16 - a_{i,j}b_{i,j})$$
$$\Delta b_{i,j} = D_b(b_{i+1,j} + b_{i-1,j} + b_{i,j+1} + b_{i,j-1} - 4b_{i,j}) + k(a_{i,j}b_{i,j} - b_{i,j} - 12 - \beta_{i,j})$$

Valleys in one dimensional case, take the form of spots in two dimensions [Figure 3] and one can obtain patterns similar to that are found on animal coats. In this project, we used the equations given above to generate two dimensional patterns and observe the effect of parameters on the resulting patterns.

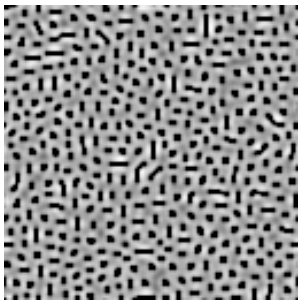


Figure 3. Two dimensional example of reaction diffusion. Concentration of b. D_a=0.1, D_b=0.02 k=0.02, B_i=0.1

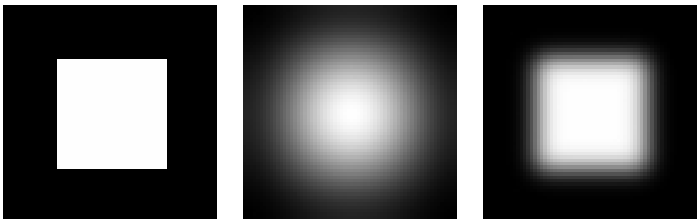
REACTION-DIFFUSION SIMULATOR

In order to perform experiments, we developed a simple reaction-diffusion simulator in Borland C++ Builder. This allowed us to easily play with the parameters and see their effect. The simulator supports both Turing and Gray-Scott model (Xmorphia, see History of RD section) of reaction-diffusion. All patterns in this report are generated using two dimensional discrete form given above with an additional constraint over concentration of morphogens – they are not allowed to take negative values to prevent numerical overflow.

Figure 4 - Reaction-Diffusion simulator

EXPERIMENTS

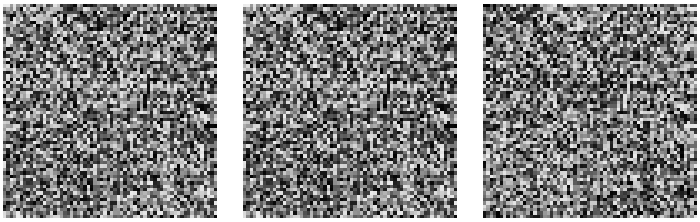
For the trivial case when k=0 (i.e. there is no reaction), the equations reduce to linear diffusion [Figure 5].



(a) (b) (c)

Figure 5. No reaction case. D_a=0.1, D_b=0.02 k=0, B_i=0.1
(a) Initial concentration, (b) morphogen a, (c) morphogen b. a is smoother since diffusion rate is larger.

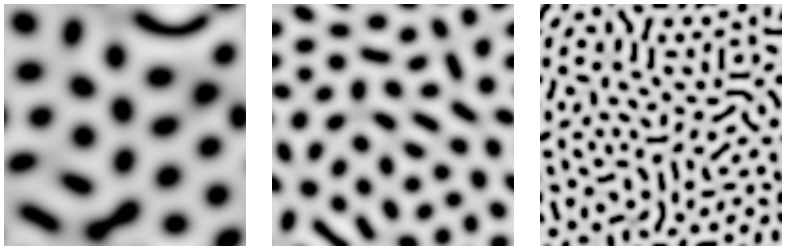
When both D_a and D_b are 0 (i.e. there is no diffusion), the concentrations of morphogens depend only on the amount of morphogens a and b already in the cell. Even though stable state might be reached, no meaningful pattern is obtained [Figure 6], because absence of diffusion precludes utilization of any spatial information.



(a) (b) (c)

Figure 6. No diffusion case. D_a= D_b=0, k=0.01, B_i=0.1.
(a) initial concentration, after 1000 (b) and 2000 (c) iterations

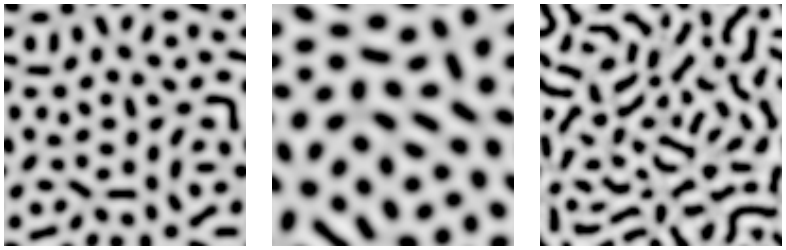
Small values for k cause the reaction part of the system to proceed more slowly relative to the diffusion, and this creates larger and more separated spots. Conversely, larger values for k produce smaller spots. [Figure 7]



k=0.001 k=0.005 k=0.01

Figure 7. The slower the reaction, the larger the spot size. D_a=0.1, D_b=0.02 k=0, B_i=0.1

If the amounts of random perturbations (β_i values) are increased, during the simulation, spots tend to join with each other and form more irregular shapes. [Figure 8]



B=0.05 B=0.1 B=3

Figure 8. More perturbation results in more irregular shapes. D_a=0.1, D_b=0.02 k=0, B_i=0.1

The joint effect of reaction rate and random perturbations are given in Figure 9.

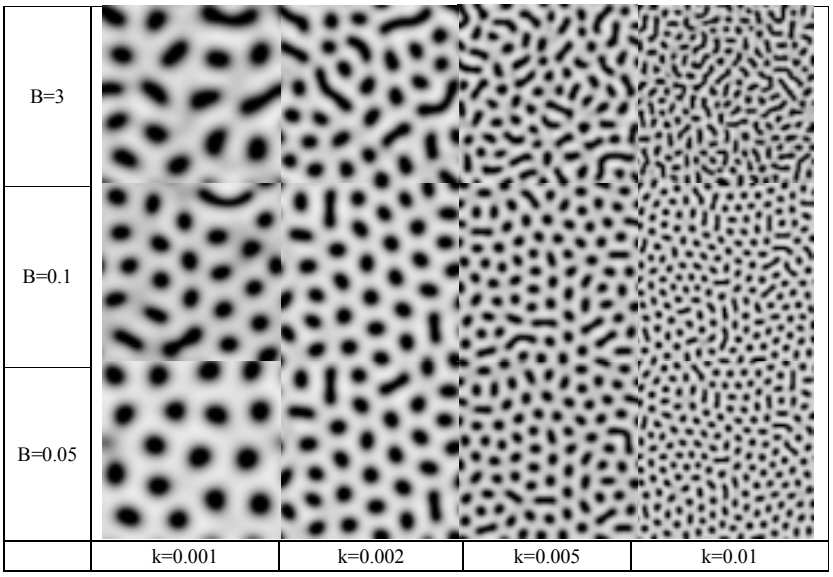


Figure 9. Reaction rate (k) vs. random perturbations (B). D_a=0.1, D_b=0.02

As D_a/D_b ratio increases, more stripe-like patterns are generated. The width of the stripes depend on the diffusion rates and the reaction speed. [Figure 10 and 11]

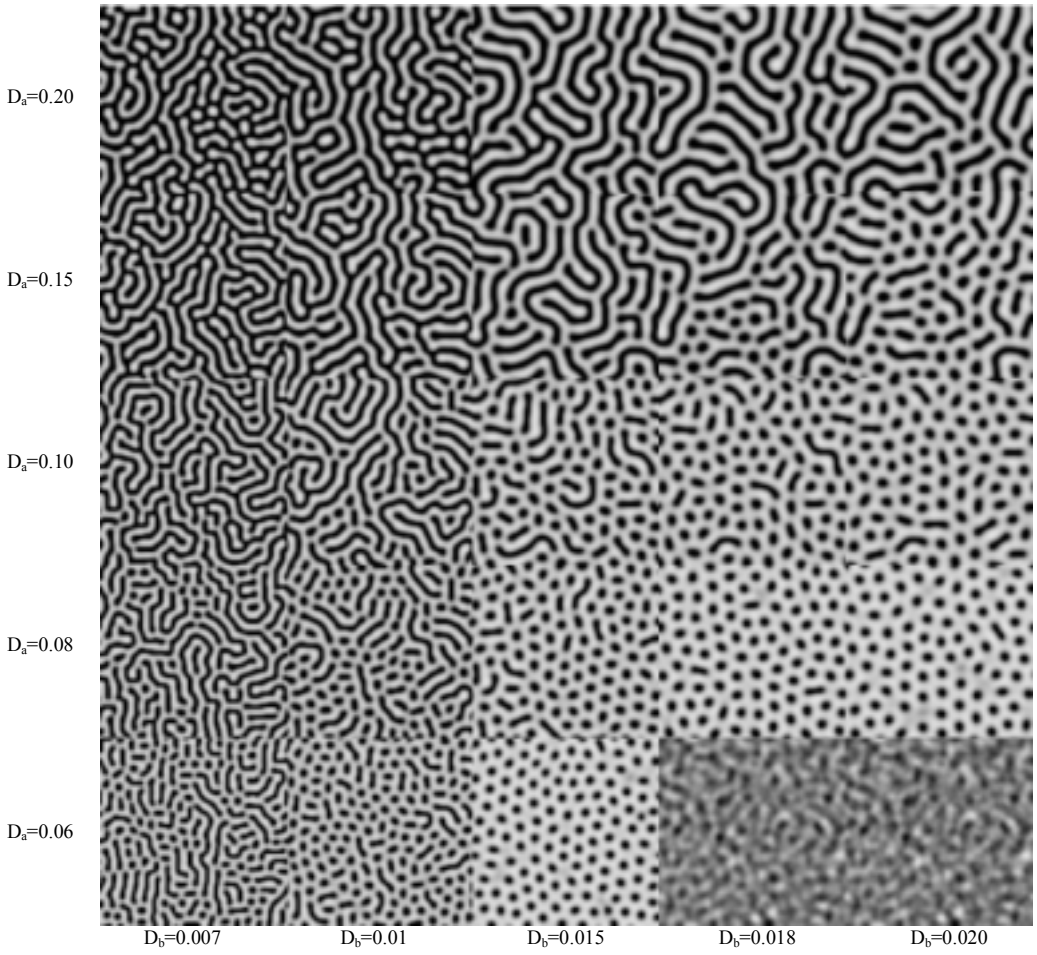


Figure 10. Varying the diffusion rates. D_a vs. D_b. k=0.005, B=0.1

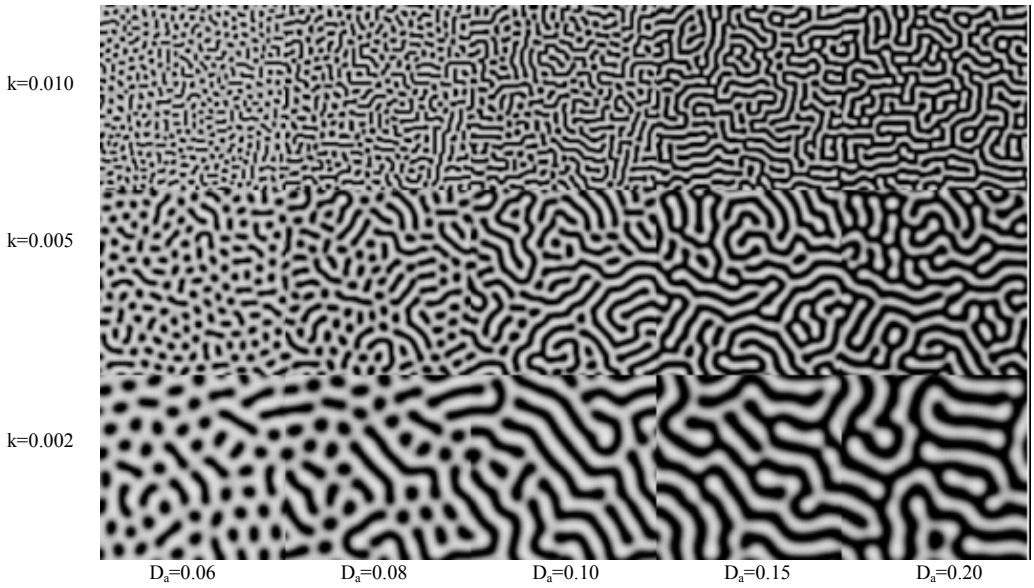


Figure 11. Reaction rate (k) vs. Diffusion rate of a (D_a). D_b=0.01, B=0.1

Using a single reaction-diffusion, we can only generate simple spot and stripe patterns. Inspired from a previous work of Bard, Turk proposed a method called *cascading* to generate more complex patterns such as jaguar coat, dark spots surrounded either by a dark ring or a circle of spots. In cascading, several reaction-diffusion systems with different parameters are run sequentially. The pattern generated using one system (after some post-processing) is used as the initial pattern of the consecutive system. For example, to obtain a cheetah pattern, following Turk's recipe, we first run our simulation with a small reaction rate (k=0.001) to obtain large spots, mark the cells whose concentration of b is between 0 and 4, and then run a new simulation with a larger reaction rate (k=0.01) in which only unmarked cells are allowed to change their concentration. Results that we obtain are given in Figure 12.

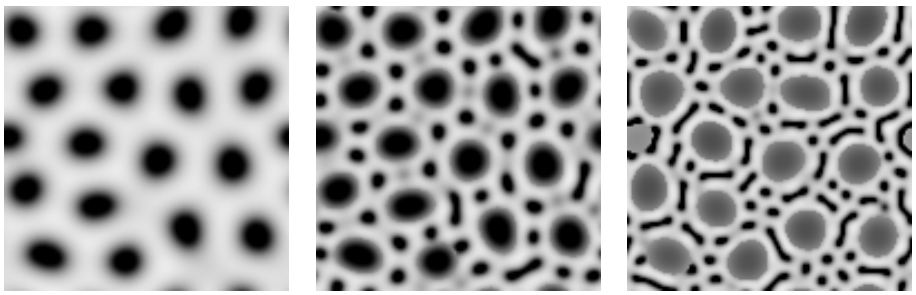


Figure 12. Cascading. D_a=0.1, D_b=0.02, B=0.05, (a) Large spot pattern generated using k=0.001, (b) Cheetah pattern. After freezing the cells with $0 \leq b \leq 4$, and running a new simulation using k=0.01, (c) Leopard pattern. At freezing stage, the concentration of b is set to 4 for the cells with, and a new simulation performed using k=0.01

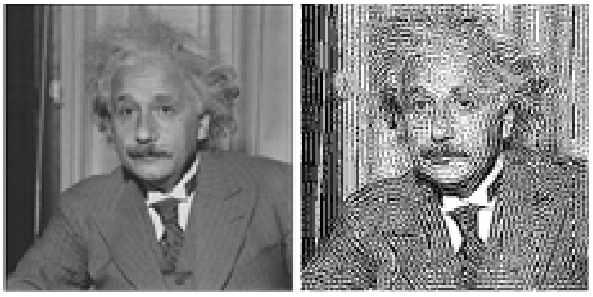
DISCUSSION

We have presented an exploration of the possible patterns obtainable by reaction-diffusion of two substrates. We believe that our experiments faithfully sample the patterns generated within the small range stability. However, it must be noted that this is by no means a complete determination of results of reaction and diffusion. The RD scheme we have used in this study is only one of many systems using the partial-differential equations (1) as the basis. In particular, different reaction terms may be used to lend the system a different behavior, and thus, resulting in different patterns.

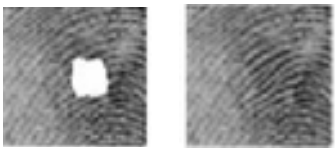
We have kept the set of parameters to be constant. for each cell, throughout each simulation. One could also vary each parameter dynamically across space and time, to obtain more complicated patterns. As with our system, it is difficult to foresee beforehand, what patterns would be generated; any claim about the results would demand a simulation of the system.

A CHRONOLOGY OF ADVANCES IN REACTION-DIFFUSION IN PATTERN GENERATION AND IMAGE PROCESSING

- 1952: Turing's landmark paper
- 1974: Bard and Launder argued that patterns generated by reaction-diffusion are not regular enough to explain patterns in development and it can explain less regular patterns such as leaf organization and distribution of hair follicles.
- 1981: Bard and Murray independently proposed use of reaction-diffusion to generate patterns on coats of animals.
- 1982: Meinhart used a reaction-diffusion system which contains 5 different morphogens to generate complex stripe patterns and presents a system that creates patterns much like the veins on a leaf.
- 1984: Young demonstrated that irregular striped patterns, similar to ocular dominance columns in mammalian visual system, can be created by reaction-diffusion.
- 1987: Meinhart and Klinger proposed that reaction-diffusion systems may explain the patterns of pigment found on mollusc shells.
- 1991: Turk used cascading to generate clusters of spots on leopards and jaguars. He also mapped these patterns over arbitrary surfaces. Whitkin and Kass extended traditional reaction-diffusion systems by allowing anisotropic and spatially non-uniform diffusion using diffusion maps.
- 1993: Pearson determined the parameter-constraints and generated a well-defined map of possible forms of patterns obtainable using Gray-Scott model. (Roy Williams later implemented a version of this system in XMorphia.)
- 1994: Sherstinsky and Picard presented "M-lattice system" which is rooted in the reaction-diffusion model and applied their model to image-restoration and orientation sensitive half toning.



- 2001: Acton, Mukherjee, Havlicek and Bovik used reaction-diffusion in reconstruction of large missing regions of homogeneous oriented textures.



Occluded Restored

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WEB RESOURCES

- Code Zebra (collection of RD links) *http://www.codezebra.net/zebraSite/archive.html*
- Greg Turk's home page
  http://www.gvu.gatech.edu/people/faculty/greg.turk/reaction_diffusion/reaction_diffusion.html
- Xmorphia *http://www.cacr.caltech.edu/ismap/image.html*
- 3D images *http://www.cs.utah.edu/~gk/papers/tvcg00/node7.html*
- Visual models of morphogenesis *http://www.cpsc.ucalgary.ca/Research/bmv/*
- Reaction-Diffusion simulator http://menekse.ceng.metu.edu.tr/Ceng/566/RD/