Homology of the Gray-Scott Model of Reaction-Diffusion

A Thesis

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Introduction

The study of pattern formation is incredibly diverse. Scientists from many disciplines have analyzes patterns on the scale of the entire universe all the way down to the microscopic[1]. Just a cursory glance at the structure of a wind-swept sand dune, a snowflake, or even our own galaxy reveals something interesting. Observation of these patterns might lead a scientist to ask what causes the pattern and wonder why there are patterns at all. This question gets complicated quickly because whether it's God in the patterns or the result of a non-equilibrium universe, there is still the question of what it means to have "structure" or "complexity" or to be "interesting".

Fortunately, the theoretical model of pattern formation discussed here allows me to sidestep all of these questions while focusing primarily on the method of analysis. There are many mathematical tools available to help understand pattern formation but applying new methods and techniques is essential, especially when analyzing a tired system like the Gray-Scott model.

[1] See the introduction of Cross & Greenside for an overview of the study of pattern formation.

Chapter 1

Reaction-Diffusion Systems

Reaction-diffusion (RD) systems are merely models that determine how concentrations of substances change in space. These systems are driven by two processes: chemical reaction and spatial diffusion. RD systems are partial differential equations, the most basic of which might look something like (1.1). This is sometimes called the Kolmogorov-Petrovsky-Piskounov equation in which u is a generic chemical species, d is a diffusion coefficient, $\nabla^2 u$ is the Laplace operator, and $r(u)$ is a general reaction term.

$$\frac{\partial u}{\partial t} = d\nabla^2 u + r(u) \tag{1.1}$$

What makes RD systems interesting, however, is the wide variety of patterns they form and how many of those patterns resemble patterns of nature such as spirals, stripes, and spots. In 1952, Alan Turing suggested that RD systems of morphogens may be able to explain the presence of spots or stripes on an organism **?**. Although the science behind animal patterns is more complicated, Turing laid the framework by which patterns form from minor perturbations of otherwise homogenous systems. Since then, many others have noted the similarity between RD patterns and patterns in nature[1].

1.1 The Gray-Scott Model

The Gray-Scott system models the reaction of two generic chemical species, U and V, whose concentration in space is represented by u and v respectively. The model

[1] Among others, Bard, 1974 or 1981; Murray, 1981; Meinhardt, 1982; Young, 1984; Meinhardt and Klinger, 1987; or Turk, 1991.

is based on the chemical reaction in (1.2).

$$\begin{aligned} U + 2V &\rightarrow 3V \\ V &\rightarrow P \end{aligned} \tag{1.2}$$

V is converted to inert product, P, which doesn't interfere with the reaction of the system. V appears on both sides of the chemical reaction and thus catalyzes its own production. Gray, Scott developed the following non-dimensional PDE:

$$\frac{\partial u}{\partial t} = d_u \nabla^2 u - uv^2 + f(1-u) \tag{1.3}$$

$$\frac{\partial v}{\partial t} = d_v \nabla^2 v + uv^2 - (f+k)v \tag{1.4}$$

We see that both equations take the form of (1.1) only they are coupled. For simplicity, d_u, d_v, f, and k are taken to be constants. The first term in each equation, $d_u \nabla^2$ and $d_v \nabla^2$, are the diffusion terms. The Laplace operator, ∇^2, is responsible for the diffusion of each chemical in space (like the diffusion of heat in the more familiar heat equation) while the *diffusion coefficients*, d_u and d_v, govern the rate. The $\pm uv^2$ term is the *reaction term* which converts U into V: an increase in v is equal to the decrease in u, hence $+uv^2$ in the second equation. Since U will eventually get used up to generate V, the term $f(1-u)$ is the *replenishment term* which reintroduces chemical U into the system (u has a maximum value of 1). Similarly, chemical V would increase without limit except for the *diminishment term*, $(f+k)v$, which serves to remove chemical V from the system. One can imagine this system as two chemicals interacting in a cell where the bloodstream carries chemicals in and out.

Chapter 2

Computational Homology

Homology is one way of analyzing *local* properties in order to extract information about *global* phenomenon. As large amounts of data become available, it becomes more difficult to determine what information is relevant. There are, of course, high and low-level approaches. A high-level approach like a fingerprint scanner or handwriting recognition might be the end-goal of one's analysis, but lower-level approaches like homology look at the geometric makeup of an object and is often a requisite step toward building higher-level processes.

At this time, computational homology is a relatively new field and its application in physics has only recently been explored. Although homology is a field of algebraic topology, it combines the mathematics of several other fields including combinatorics and computation. The mathematical formalism behind homology is difficult to grasp so only the relevant information will be detailed here.

2.1 Image analysis

To put it simply, homology is concerned with *holes* and *pieces*. Mathematically, how does one define a "hole"? What does it mean to be part of a "connected piece"? It's best to think about this in one dimension first. Figure 2.1 shows two simple topological spaces, X and Y. Although X and Y are spaces with one and two line segments respectively, in terms of homology one would say X consists of a single *connected piece* while Y has two distinct pieces. The fact that the line segments are straight or of different length is not important for the homology. In this one-dimensional example, the *zeroth homology groups* of each are

$$H_0(X) \cong \mathbf{Z}^1 \qquad \text{and} \quad H_0(Y) \cong \mathbf{Z}^2 \tag{2.1}$$

where $\mathbf{Z}$ is the group of integers. The homology pairs a topological space (e.g.

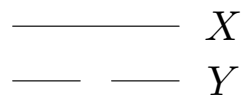

Figure 2.1: Topological spaces X and Y. X consists of one connected line segment and Y has two disconnected line segments.

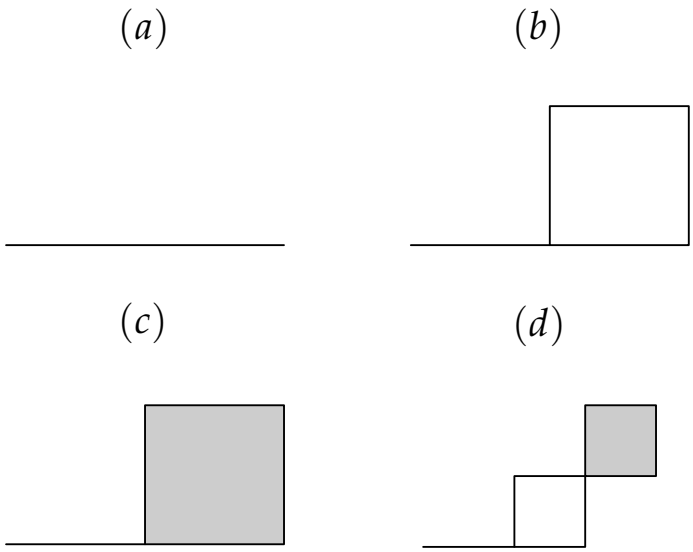

Figure 2.2: Topological spaces X_a, X_b, X_c, and X_d.

X and Y) with an *abelian group*, a set of elements combined with operations that satisfy five axioms (closure, associativity, identity, invertibility, and commutativity). Notice, however, that the *zeroth homology grou*p of Y is $\mathbf{Z}^2$; the exponent, 2, is what accounts for the two (2) distinct pieces, but more on this later.

Since there is a *zeroth homology group*, it makes sense that there would be a *first homology group*. Looking at the two-dimensional example in Figure 2.2, the homology of each space X_a, X_b, X_c, and X_d is

$$H_1(X_a) \cong 0 \quad H_1(X_b) \cong \mathbf{Z} \qquad H_1(X_c) \cong 0 \quad H_1(X_d) \cong \mathbf{Z} \tag{2.2}$$

$$H_0(X_i) \cong \mathbf{Z} \qquad \text{for} \qquad i = a, b, c, d \tag{2.3}$$

All spaces X_i for $i = a, b, c, d$ have a *zeroth homology group* of $\mathbf{Z}$ since there is a single connected component. In Figure 2.2(b)-(c), the connected component forms an enclosed area (e.g. the squares). The square in (b) forms a "hole". The shading indicates that the hole is filled and is thus no longer a "hole". Figure 2.3(b), (d) both contain one hole while (a), (c) contain zero holes. Just as the *zeroth homology group* is concerned with connected segments, the *first homology group* is concerned

with "holes".

The terms "piece" and "hole" are informal. Formally, we could say that the k^{th} homology group, $H_k(X)$, represents the k-dimensional *holes* of X where a 0-dimensional *hole* is merely the gap between two components (e.g. Y in figure 2.1).

Chapter 3

Mathematics and Science

3.1 Math

TEX is the best way to typeset mathematics. Donald Knuth designed TEX when he got frustrated at how long it was taking the typesetters to finish his book, which contained a lot of mathematics.

If you are doing a thesis that will involve lots of math, you will want to read the following section which has been commented out. If you're not going to use math, skip over this next big red section. (It's red in the .tex file but does not show up in the .pdf.)

$$\sum_{j=1}^{n}(\delta\theta_j)^2 \leq \frac{\beta_i^2}{\delta_i^2+\rho_i^2}\left[2\rho_i^2+\frac{\delta_i^2\beta_i^2}{\delta_i^2+\rho_i^2}\right] \equiv \omega_i^2$$

From Informational Dynamics, we have the following (Dave Braden):
After n such encounters the posterior density for θ is

$$\pi(\theta|X_1 < y_1, \ldots, X_n < y_n) \propto \pi(\theta)\prod_{i=1}^{n}\int_{-\infty}^{y_i}\exp\left(-\frac{(x-\theta)^2}{2\sigma^2}\right)\,dx$$

Another equation:

$$\det\begin{vmatrix} c_0 & c_1 & c_2 & \ldots & c_n \\ c_1 & c_2 & c_3 & \ldots & c_{n+1} \\ c_2 & c_3 & c_4 & \ldots & c_{n+2} \\ \vdots & \vdots & \vdots & & \vdots \\ c_n & c_{n+1} & c_{n+2} & \ldots & c_{2n} \end{vmatrix} > 0$$

Lapidus and Pindar, Numerical Solution of Partial Differential Equations in Science and Engineering. Page 54

$$\int_t \left\{ \sum_{j=1}^{3} T_j \left(\frac{d\phi_j}{dt} + k\phi_j \right) - kT_e \right\} w_i(t)\, dt = 0, \qquad i = 1, 2, 3.$$

L&P Galerkin method weighting functions. Page 55

$$\sum_{j=1}^{3} T_j \int_0^1 \left\{ \frac{d\phi_j}{dt} + k\phi_j \right\} \phi_i\, dt = \int_0^1 k\, T_e \phi_i dt, \qquad i = 1, 2, 3$$

Another L&P (p145)

$$\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} f(\xi, \eta, \zeta) = \sum_{k=1}^{n}\sum_{j=1}^{n}\sum_{i=1}^{n} w_i w_j w_k f(\xi, \eta, \zeta).$$

Another L&P (p126)

$$\int_{A_e} (\,\cdot\,) dx dy = \int_{-1}^{1}\int_{-1}^{1} (\,\cdot\,) \det[J] d\xi d\eta.$$

3.2 Chemistry 101: Symbols

Chemical formulas will look best if they are not italicized. Get around math mode's automatic italicizing by using the argument `$\mathrm{formula here}$`, with your formula inside the curly brackets.

So, $Fe_2^{2+}Cr_2O_4$ is written `$\mathrm{Fe_2^{2+}Cr_2O_4}$`
Exponent or Superscript: O^-
Subscript: CH_4

To stack numbers or letters as in Fe_2^{2+}, the subscript is defined first, and then the superscript is defined.
Angstrom: Å
Bullet: $CuCl \bullet 7H_2O$
Double Dagger: ‡
Delta: Δ
Reaction Arrows: $\longrightarrow$ or $\xrightarrow{solution}$
Resonance Arrows: $\leftrightarrow$
Reversible Reaction Arrows: $\rightleftharpoons$ or $\xrightleftharpoons{solution}$ (the latter requires the chemarr package)

3.2.1 Typesetting reactions

You may wish to put your reaction in a figure environment, which means that LaTeX will place the reaction where it fits and you can have a figure legend if

desired:

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

Figure 3.1: Combustion of glucose

3.2.2 Other examples of reactions

$NH_4Cl_{(s)} \rightleftharpoons NH_{3(g)} + HCl_{(g)}$

$MeCH_2Br + Mg \xrightarrow[below]{above} MeCH_2 \bullet Mg \bullet Br$

3.3 Physics

Many of the symbols you will need can be found on the math page (`http://web.reed.edu/cis/help/latex/math.html`) and the Comprehensive LaTeX Symbol Guide (enclosed in this template download). You may wish to create custom commands for commonly used symbols, phrases or equations, as described in Chapter **??**.

3.4 Biology

You will probably find the resources at `http://www.lecb.ncifcrf.gov/~toms/latex.html` helpful, particularly the links to bsts for various journals. You may also be interested in TeXShade for nucleotide typesetting (`http://homepages.uni-tuebingen.de/beitz/txe.html`). Be sure to read the proceeding chapter on graphics and tables, and remember that the thesis template has versions of Ecology and Science bsts which support webpage citation formats.

Chapter 4

Tables and Graphics

4.1 Tables

The following section contains examples of tables, most of which have been commented out for brevity. (They will show up in the .tex document in red, but not at all in the .pdf). For more help in constructing a table (or anything else in this document), please see the LaTeX pages on the CUS site.

Table 4.1: A Basic Table: Correlation of Factors between Parents and Child, Showing Inheritance

Factors	Correlation between Parents & Child	Inherited
Education	-0.49	Yes
Socio-Economic Status	0.28	Slight
Income	0.08	No
Family Size	0.19	Slight
Occupational Prestige	0.21	Slight

If you want to make a table that is longer than a page, you will want to use the longtable environment. Uncomment the table below to see an example, or see our online documentation.

Table 4.2: An example of a long table, with headers that repeat on each subsequent page: Results from the summers of 1998 and 1999 work at Reed College done by Grace Brannigan, Robert Holiday and Lien Ngo in 1998 and Kate Brown and Christina Inman in 1999.

Chromium Hexacarbonyl			
State	Laser wavelength	Buffer gas	Ratio of $\frac{\text{Intensity at vapor pressure}}{\text{Intensity at 240 Torr}}$
$z^7P_4^\circ$	266 nm	Argon	1.5
$z^7P_2^\circ$	355 nm	Argon	0.57
$y^7P_3^\circ$	266 nm	Argon	1
$y^7P_3^\circ$	355 nm	Argon	0.14
$y^7P_2^\circ$	355 nm	Argon	0.14
$z^5P_3^\circ$	266 nm	Argon	1.2
$z^5P_3^\circ$	355 nm	Argon	0.04
$z^5P_3^\circ$	355 nm	Helium	0.02
$z^5P_2^\circ$	355 nm	Argon	0.07
$z^5P_1^\circ$	355 nm	Argon	0.05
$y^5P_3^\circ$	355 nm	Argon	0.05, 0.4
$y^5P_3^\circ$	355 nm	Helium	0.25
$z^5F_4^\circ$	266 nm	Argon	1.4
$z^5F_4^\circ$	355 nm	Argon	0.29
$z^5F_4^\circ$	355 nm	Helium	1.02
$z^5D_4^\circ$	355 nm	Argon	0.3
$z^5D_4^\circ$	355 nm	Helium	0.65
$y^5H_7^\circ$	266 nm	Argon	0.17
$y^5H_7^\circ$	355 nm	Argon	0.13
$y^5H_7^\circ$	355 nm	Helium	0.11
a^5D_3	266 nm	Argon	0.71
a^5D_2	266 nm	Argon	0.77
a^5D_2	355 nm	Argon	0.63
a^3D_3	355 nm	Argon	0.05
a^5S_2	266 nm	Argon	2
a^5S_2	355 nm	Argon	1.5
a^5G_6	355 nm	Argon	0.91
a^3G_4	355 nm	Argon	0.08

State	Laser wavelength	Buffer gas	Ratio of $\frac{\text{Intensity at vapor pressure}}{\text{Intensity at 240 Torr}}$
e^7D_5	355 nm	Helium	3.5
e^7D_3	355 nm	Helium	3
f^7D_5	355 nm	Helium	0.25
f^7D_5	355 nm	Argon	0.25
f^7D_4	355 nm	Argon	0.2
f^7D_4	355 nm	Helium	0.3
Propyl-ACT			
$z^7P_4^\circ$	355 nm	Argon	1.5
$z^7P_3^\circ$	355 nm	Argon	1.5
$z^7P_2^\circ$	355 nm	Argon	1.25
$z^7F_5^\circ$	355 nm	Argon	2.85
$y^7P_4^\circ$	355 nm	Argon	0.07
$y^7P_3^\circ$	355 nm	Argon	0.06
$z^5P_3^\circ$	355 nm	Argon	0.12
$z^5P_2^\circ$	355 nm	Argon	0.13
$z^5P_1^\circ$	355 nm	Argon	0.14
Methyl-ACT			
$z^7P_4^\circ$	355 nm	Argon	1.6, 2.5
$z^7P_4^\circ$	355 nm	Helium	3
$z^7P_4^\circ$	266 nm	Argon	1.33
$z^7P_3^\circ$	355 nm	Argon	1.5
$z^7P_2^\circ$	355 nm	Argon	1.25, 1.3
$z^7F_5^\circ$	355 nm	Argon	3
$y^7P_4^\circ$	355 nm	Argon	0.07, 0.08
$y^7P_4^\circ$	355 nm	Helium	0.2
$y^7P_3^\circ$	266 nm	Argon	1.22
$y^7P_3^\circ$	355 nm	Argon	0.08
$y^7P_2^\circ$	355 nm	Argon	0.1
$z^5P_3^\circ$	266 nm	Argon	0.67
$z^5P_3^\circ$	355 nm	Argon	0.08, 0.17
$z^5P_3^\circ$	355 nm	Helium	0.12
$z^5P_2^\circ$	355 nm	Argon	0.13
$z^5P_1^\circ$	355 nm	Argon	0.09
$y^5H_7^\circ$	355 nm	Argon	0.06, 0.05
a^5D_3	266 nm	Argon	2.5
a^5D_2	266 nm	Argon	1.9
a^5D_2	355 nm	Argon	1.17
a^5S_2	266 nm	Argon	2.3

State	Laser wavelength	Buffer gas	Ratio of $\frac{\text{Intensity at vapor pressure}}{\text{Intensity at 240 Torr}}$
a^5S_2	355 nm	Argon	1.11
a^5G_6	355 nm	Argon	1.6
e^7D_5	355 nm	Argon	1

4.2 Figures

If your thesis has a lot of figures, LaTeX might behave better for you than that other word processor. One thing that may be annoying is the way it handles "floats" like tables and figures. LaTeX will try to find the best place to put your object based on the text around it and until you're really, truly done writing you should just leave it where it lies. There are some optional arguments to the figure and table environments to specify where you want it to appear; see the comments in the first figure.

If you need a graphic or tabular material to be part of the text, you can just put it inline. If you need it to appear in the list of figures or tables, it should be placed in the floating environment.

To get a figure from StatView, JMP, SPSS or other statistics program into a figure, you can print to pdf or save the image as a jpg or png. Precisely how you will do this depends on the program: you may need to copy-paste figures into Photoshop or other graphic program, then save in the appropriate format.

Below we have put a few examples of figures. For more help using graphics and the float environment, see our online documentation.

And this is how you add a figure with a graphic:

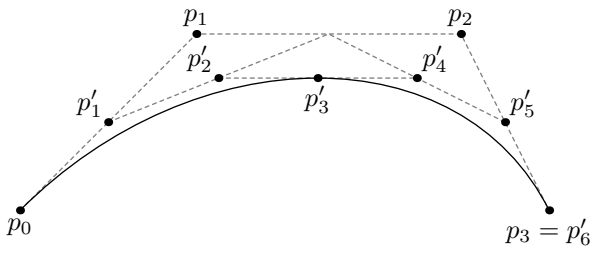

Figure 4.1: A Figure

4.3 More Figure Stuff

You can also scale and rotate figures.

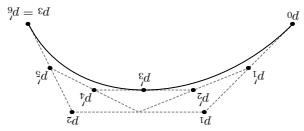

Figure 4.2: A Smaller Figure, Flipped Upside Down

4.4 Even More Figure Stuff

With some clever work you can crop a figure, which is handy if (for instance) your EPS or PDF is a little graphic on a whole sheet of paper. The viewport arguments are the lower-left and upper-right coordinates for the area you want to crop.

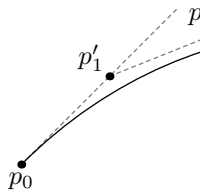

Figure 4.3: A Cropped Figure

4.4.1 Common Modifications

The following figure features the more popular changes thesis students want to their figures. This information is also on the web at `web.reed.edu/cis/help/latex/graphics.html`.

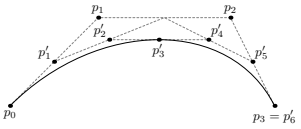

Figure 0.8: Interaction bar plot showing the degree of specialization for each flower type.

Conclusion

Here's a conclusion, demonstrating the use of all that manual incrementing and table of contents adding that has to happen if you use the starred form of the chapter command. The deal is, the chapter command in LaTeX does a lot of things: it increments the chapter counter, it resets the section counter to zero, it puts the name of the chapter into the table of contents and the running headers, and probably some other stuff.

So, if you remove all that stuff because you don't like it to say "Chapter 4: Conclusion", then you have to manually add all the things LaTeX would normally do for you. Maybe someday we'll write a new chapter macro that doesn't add "Chapter X" to the beginning of every chapter title.

4.1 More info

And here's some other random info: the first paragraph after a chapter title or section head *shouldn't be* indented, because indents are to tell the reader that you're starting a new paragraph. Since that's obvious after a chapter or section title, proper typesetting doesn't add an indent there.

Appendix A

The First Appendix

An appendix full of awesome

Appendix B

The Second Appendix, for Fun

An appendix full of win