

## Abstract

This project investigates the Gray-Scott model for replicating patterns found in nature using numerical methods and standard non-linear analysis. The Gray-Scott model is investigated and applied using standard parameters. Pattern formation was successfully observed and the effectiveness of the models use in forming biological patterns is discussed.

## Introduction

Most systems in nature are non-linear. Mathematical models with the aid of computational techniques are designed to mimic the rules that govern the dynamics of biological, physical or chemical systems which exhibit non-linear behaviour. An example of such a system is the Gray-Scott model, which is used to simulate a reaction-diffusion system. The model consists of two chemical species which interact according to the following equation:  $U + 2V \rightarrow 3V$ , where  $U$  is the concentration of the reactant and  $V$  is the concentration of the catalyst.

Applications of the Gray-Scott model in biological systems include the growth of bacterial colonies, the patterns of spots and stripes in animals, and the development of plant roots.

To find a homogenous state for the system we set,  $\frac{dU}{dt} = \frac{dV}{dt} = \nabla^2 U = \nabla^2 V = 0$  the fixed points emerging are:

►  $U = 1, V = 0$ .

For  $0 < k < \frac{1}{2}(\sqrt{F} - 2F)$ ,  $0 < F < \frac{1}{4}$  the following fixed points emerge:

- $U_+ = \frac{1}{2}\left(1 + \sqrt{1 - \frac{4(F+k)^2}{F}}\right)$ .  $V_- = \frac{1}{2F+k}\left(1 - \sqrt{1 - \frac{4(F+k)^2}{F}}\right)$ .
- $U_- = \frac{1}{2}\left(1 - \sqrt{1 - \frac{4(F+k)^2}{F}}\right)$ .  $V_+ = \frac{1}{2F+k}\left(1 + \sqrt{1 - \frac{4(F+k)^2}{F}}\right)$ .

To classify the fixed point, we consider a small perturbation  $k_1, k_2$  about the homogenous states ( $U_h, V_h$ ):

- $U(x, y, t) = U_h + k_1(x, y, t)$ ,
- $V(x, y, t) = V_h + k_2(x, y, t)$ .

The linearised equations governing perturbations are:

$$\frac{dk_1}{dt} = (-V^2 - F)k_1 - 2UVk_2 + D_u\nabla^2 k_1,$$

$$\frac{dk_2}{dt} = V^2k_1 + (2UV - (F + k))k_2 + D_v\nabla^2 k_2.$$

## Computational Techniques

We try to solve the model numerically using the method of finite differences followed by Euler integration. First and second order derivative of a function  $f(x)$  can be approximated using:

$$f'(x) \sim \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}, \quad f''(x) \sim \lim_{h \rightarrow 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

If we consider a step size  $h$  in the spatial domain,

$$\begin{aligned} \frac{dU}{dt} &\sim D_u \frac{U(x+h, y, t) - 4U(x, y, t) + U(x-h, y, t) + U(x, y+h, t) + U(x, y-h, t)}{h^2} \\ &\quad + U(x, y, t)V(x, y, t)^2 + F(1 - U(x, y, t)) \end{aligned}$$

to find the value of  $U$  for the next increment of time, we use

$$U(t + dt, x, y) \sim \frac{dU}{dt} dt + U(x, y, t)$$

where  $dt = 1$ . The same procedure is carried out for  $V(t + dt, x, y)$ . The iterative process is carried everywhere except at the edges of the grid so that periodic boundary conditions can be applied. The initial conditions used were:  $(U = 2 * 10^{-5}, V = 1 * 10^{-5})$  with  $\frac{D_u}{D_v} = 2$ , to simulate the time evolution of reactant and catalyst concentration in the spatial domain using contour plots with varying  $F$  and  $k$  parameters.

## Discussion and Conclusion

Using the ratio  $D_u/D_v$  being equal to 2 allowed the formation of patterns of self-replicating spots, worm-like patterns as well as temporal chaos where the pattern was no longer predictable over time. When the ratio of diffusion coefficients was set to 1 however, the dynamic evolution of the system was similar to a radial wave going inwards or outwards with the system conserving its symmetric properties. For the method of finite differences, we have an error of  $O(h^2)$  for the spatial step and an error of  $O(dt)$  for the time step. This method is suitable for the square geometry chosen for our experiment, but finite volume methods could explore systems with more complicated geometries.

## Theory

The Gray-Scott model is described by the following Partial Differential Equations (PDEs):

$$\frac{dU}{dt} = -UV^2 + F(1 - U) + D_u\nabla^2 U$$

$$\frac{dV}{dt} = +UV^2 - (F + k)V + D_v\nabla^2 V$$

where  $U$  is the concentration of the reactant,  $V$  is the concentration of the catalyst,  $F$  is the rate at which  $U$  is being replenished in the reaction (feed rate),  $k$  is the rate at which  $V$  is being removed from the reaction (kill rate),  $D_u$  is the diffusion rate of  $U$ ,  $D_v$  is the diffusion rate of  $V$ , and  $\nabla^2$  indicates the two dimensional Laplacian.

The resulting Jacobian matrix of the perturbation:

$$J = \begin{pmatrix} -V^2 - F & -2UV \\ V^2 & 2UV - (F + k) \end{pmatrix}.$$

For the homogeneous state  $(1, 0)$  the eigenvalues of the jacobian are both real and negative we have a stable node. For the  $(U_+, V_-)$  state we have a saddle point with equal magnitude eigenvalues of opposite signs. For the  $(U_-, V_+)$  state, we have a stable node for

$$F > \frac{1}{2}\left(-\sqrt{k - 4k^{\frac{3}{2}}} - 2k + \sqrt{k}\right).$$

The node turns unstable otherwise with both eigenvalues being positive. Trajectories in phase space approach attractors (stable nodes) and move away from repellers (unstable nodes). Trajectories approach the saddle point from the negative eigenvalue and move away from the positive one.

## Results

