The Gray-Scott Equations

The Gray-Scott equations are a set of coupled, partial differential equations which can be expressed as,

$$u_t = \epsilon_u \nabla^2 u - uv^2 + F(1-u), \tag{1}$$

$$v_t = \epsilon_v \nabla^2 v + uv^2 - (c+F)v. \tag{2}$$

The ∇^2 term here represents the two-dimensional Laplacian operator,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

So, we know these equations for u_t and v_t as two-dimensional, time-dependent diffusion equations with sources $-uv^2 + F(1-u)$ and $+uv^2 - (c+F)v$, respectively. The diffusion coefficients are fixed as $\epsilon_u = 5 \times 10^{-5}$ and $\epsilon_v = 2 \times 10^{-5}$, while two choices of (c, F) were investigated: $(0.065, 0.06)$ and $(0.065, 0.03)$.

2D finite differences approach

Since we have two coupled PDEs which vary in x and y, this system can be solved numerically using a 2D finite differences approach. In particular, the forward Euler method can be employed, where we can substitute approximate time and spatial derivatives for a series of discretized points (x_j, y_k, t_n). Looking at $u(x, y, t)$, for example, we have,

$$u_t \approx \frac{u_{jk}^{n+1} - u_{jk}^n}{\Delta t}, \text{ and,} \tag{3}$$

$$\nabla^2 u \approx \frac{1}{h^2} \left(u_{j+1,k}^n - 2u_{jk}^n + u_{j-1,k}^n + u_{j,k+1}^n - 2u_{jk}^n + u_{j,k-1}^n \right). \tag{4}$$

Substituting these expressions into the first PDE, and solving for u_{jk}^{n+1}, we obtain,

$$u_{jk}^{n+1} = F\Delta t + u_{jk}^n \left(1 - \frac{4\epsilon_u \Delta t}{h^2} - \Delta t((v_{jk}^n)^2 + F) \right) + \frac{\epsilon_u \Delta t}{h^2} \left(u_{j+1,k}^n + u_{j-1,k}^n + u_{j,k+1}^n + u_{j,k-1}^n \right) \tag{5}$$

We can define a constant $\lambda_u = \epsilon_u \Delta t / h^2$, so then,

$$u_{jk}^{n+1} = F\Delta t + u_{jk}^n \left(1 - 4\lambda_u - \Delta t((v_{jk}^n)^2 + F)\right) \\ + \lambda_u \left(u_{j+1,k}^n + u_{j-1,k}^n + u_{j,k+1}^n + u_{j,k-1}^n\right). \quad (6)$$

Similarly, for v_{jk}^{n+1}, we have,

$$v_{jk}^{n+1} = v_{jk}^n \left(1 - 4\lambda_v + \Delta t u_{jk}^n v_{jk}^n - c\Delta t - F\Delta t\right) \\ + \lambda_v \left(v_{j+1,k}^n + v_{j-1,k}^n + v_{j,k+1}^n + v_{j,k-1}^n\right), \quad (7)$$

where λ_v is defined equivalently as $\lambda_v = \epsilon_v \Delta t / h^2$.

It is evident from the forms of these equations that we can define a common matrix to propagate the diffusive components in u and v, with unique source terms to account for the reaction components. So, we define a matrix L using periodic boundary conditions as,

$$L = \begin{pmatrix} -2 & 1 & 0 & ... & 1 \\ 1 & -2 & 1 & ... & 0 \\ & & \vdots & \ddots & \\ 1 & 0 & ... & 1 & -2 \end{pmatrix} \quad (8)$$

such that the full, 2D diffusion matrices can be expressed using MATLAB's `kron` command, along with the $N \times N$ identity matrix I, as,

`Lx = kron(L,I); Ly = kron(I,L); II = kron(I,I)`, and, (9)

$$A_u = \mathbb{1} + \lambda_u (L_x + L_y), \quad A_v = \mathbb{1} + \lambda_v (L_x + L_y). \quad (10)$$

Then the final, vectorized expressions for $\vec{u}^{\,n+1}$ and $\vec{v}^{\,n+1}$ are,

$$\vec{u}^{\,n+1} = A_u \vec{u}^{\,n} - \vec{u}^{\,n} \circ \left(\vec{v}^{\,n} \circ \vec{v}^{\,n} + \vec{F}\right) \Delta t + \vec{F} \Delta t, \text{ and,} \quad (11)$$

$$\vec{v}^{\,n+1} = A_v \vec{v}^{\,n} + \vec{v}^{\,n} \circ \left(\vec{u}^{\,n} \circ \vec{v}^{\,n} - \vec{c} - \vec{F}\right) \Delta t. \quad (12)$$

Here, $\vec{u}^{\,n}$ and $\vec{v}^{\,n}$ are vectors of length N^2 containing information on every point u_{jk} and v_{jk} at time n within the x-y grid. Furthermore, '$\circ$' represents the Hadamard (elementwise) product of two vectors, and $\vec{F}$ and $\vec{c}$ are size N^2 vectors composed entirely of the constants F and c, respectively.

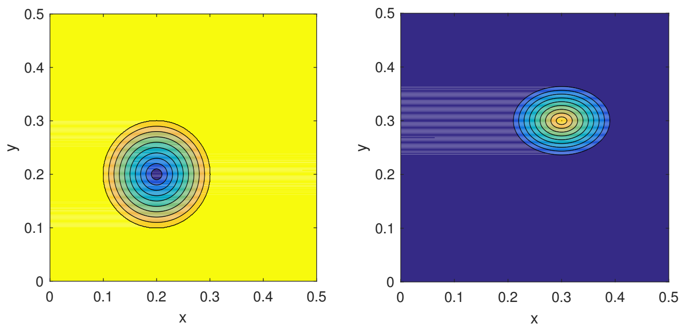


Figure 1: Conditions at $t = 0$ for the system for u (left) and v (right).

Results

The 2D finite differences method was implemented in Matlab. In order to determine whether (and to what degree) the forward Euler propagation was sensitive to choice of step size, the finite differences propagation was repeated for several choices of Δt and h, with the benchmark for agreement being the value of $u(0.25, 0.25)$ at a time $t_{\max} = 20$. The goal of this scan was to get a consistent answer of $u(0.25, 0.25)$ down to "several" decimal places, which was taken to be four (i.e. "more than two but not many"). Table 1 shows the results of this scan for different choices of Δt and h. It was found that choosing $\Delta t = h = 0.0001$ provided the required precision, as the absolute error Δu between successive iterations was $\mathcal{O}\left(10^{-5}\right)$ for each parameter set.

Using this step size configuration, the values of $u(0.25, 0.25)$ were calculated at $t_{\max} = 500$ and 3000, [1] with the results given in Table 2. Corresponding plots of $u(x, y)$ and $v(x, y)$ were produced for each (c, F) set on the same time scales, with the resultant distributions found in Figures 2 and 3 for $t_{\max} = 500$ and 3000, respectively. The effect of the periodic boundary conditions in L is immediately evident in the distributions for $t_{\max} = 500$, where the rightmost diffusion contours cut off at the edges of the figure, and re-emerge at the opposite end of the distribution.

When we compare the evolution of the system at $t_{\max} = 500$ and 3000, as well, the impact of the two choices of parameters becomes clearer. When F is larger, the impact on the removal of $u(x, y, t)$ is more visible. For example, at $t_{\max} = 500$, the system becomes clearly centred around $(0.3, 0.3)$, indicating that the v component is dominating the diffusion reaction. Likewise,

[1]Runtime for $t_{\max} = 3000$ was ~ 8 hours, so these runs were made over two successive nights of processing.

while the distribution has evolved into a more complex pattern, the diffusion effects still seem to be centred around $x = y = 0.3$. Conversely, for the case of $F = 0.03$, the diffusion patterns are more dynamic, and demonstrate a long-term interaction of the u and v components of the system. A particularly interesting behaviour visible for $F = 0.03$ is that multiple spots of small u / high v appear to spring up over time. Viewing the diffusion in real time reveals a multiplication effect where a spot will emerge, then subdivide into two spots. The net result of this multiplication is visible in the bottom of Figure 3, where 11 spots have emerged over the whole phase space, while initially only a single spot in u existed at $t = 0$.

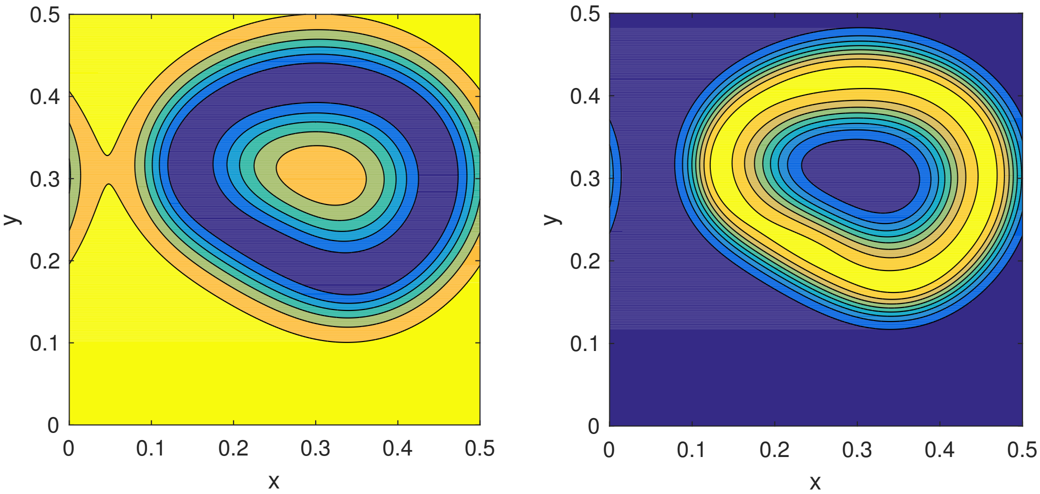
Worth noting, as well, is that the results of these diffusion equations can be compared to the results obtained by J.E. Pearson, as published in *Science* [1]. In particular, Figure 3 in Pearson's paper identifies several pattern types, and the parameter space in (c, F) in which they may be found. Although the initial conditions and ϵ terms are different than the system he defines, it is nonetheless worth making qualitative comparisons where we can. Around $(0.065, 0.03)$, Pearson finds that the system tends to evolve towards a series of spots, not unlike what is seen for $t_{\max} = 3000$ in the bottom of Figure 3. Likewise, around the region $(0.065, 0.06)$, Pearson finds that the system evolves towards a series of elongated, diagonal wells, which is also reminiscent of the final state at the top of Figure 3. Therefore, it appears that the end results of the Grey-Scott system propagation shown here are qualitatively similar to what Pearson found in his paper.

$(c, F) = (0.065, 0.06),\ t_{\max} = 20$			
Δt	h	$u(0.25, 0.25)$	Δu
0.01000	0.01000	0.40524	-
0.00500	0.00500	0.40371	0.00153
0.00200	0.00200	0.40331	0.00040
0.00100	0.00100	0.40325	0.00006
$(c, F) = (0.065, 0.03),\ t_{\max} = 20$			
Δt	h	$u(0.25, 0.25)$	Δu
0.01000	0.01000	0.27336	-
0.00500	0.00500	0.27220	0.00116
0.00200	0.00200	0.27190	0.00030
0.00100	0.00100	0.27186	0.00004

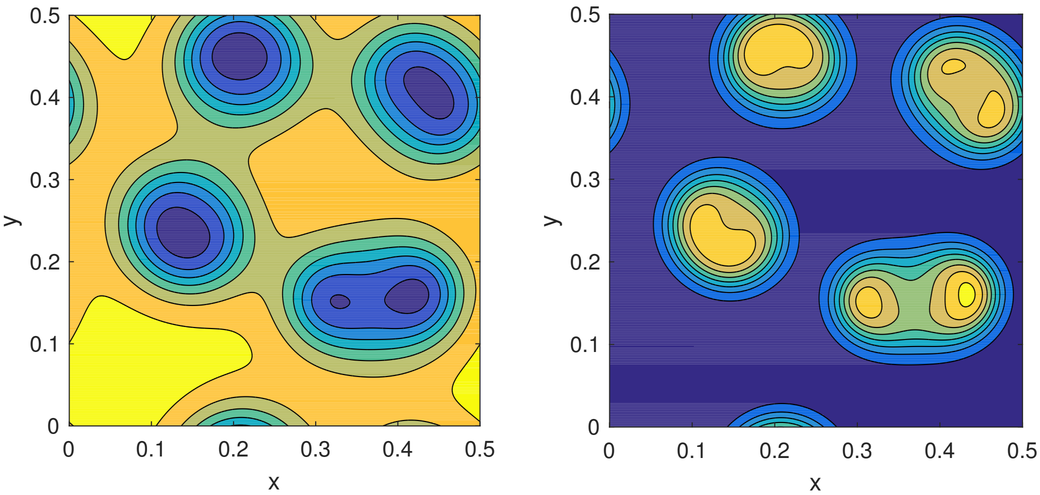
Table 1: Testing different values of Δt and h for a nominal point $u(0.25, 0.25)$ at $t_{\max} = 20$.

	Value of $u(0.25, 0.25)$	
$t_{\max}$	$(c, F) = (0.065, 0.06)$	$(c, F) = (0.065, 0.03)$
500	0.48580	0.80845
3000	0.77655	0.77095

Table 2: Values of $u(0.25, 0.25)$ at $t_{\max} = 500$ and 3000 for step sizes $\Delta t = h = 0.001$.

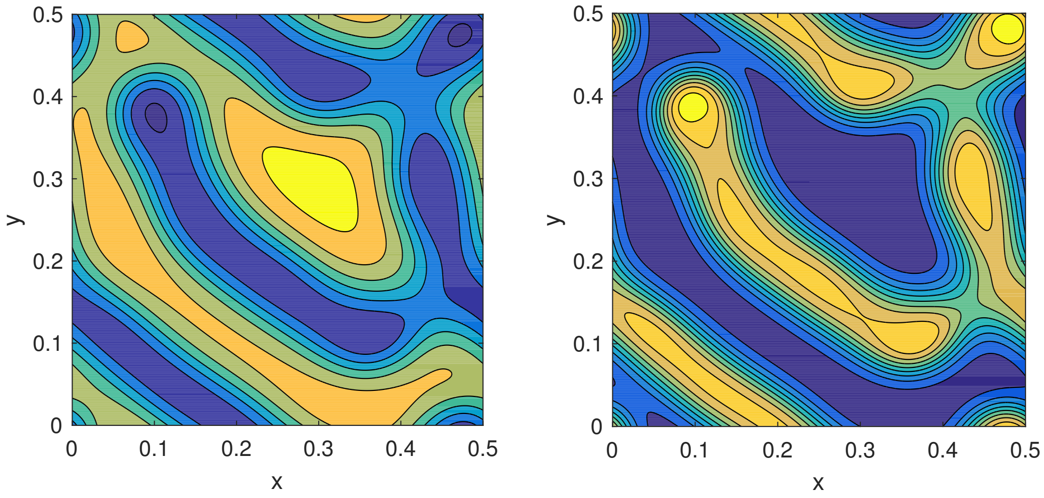


(a) $(0.065, 0.06)$, $t_{\max} = 500$

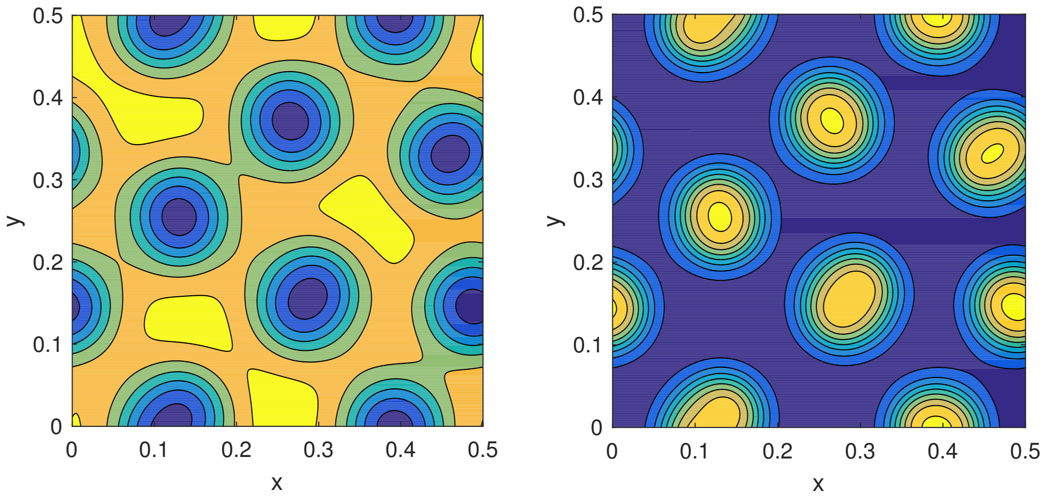


(b) $(0.065, 0.03)$, $t_{\max} = 500$

Figure 2: Conditions at $t = 500$ for the Grey-Scott system for u (left) and v (right).



(a) $(0.065, 0.06)$, $t_{\max} = 3000$



(b) $(0.065, 0.03)$, $t_{\max} = 3000$

Figure 3: Conditions at $t = 3000$ for the Grey-Scott system for u (left) and v (right).

References

[1] J. E. Pearson, *Complex Patterns in a Simple System*, Science **261** (1993) no. 5118, 189–192. http://www.staff.science.uu.nl/~frank011/Classes/complexity/Literature/Pearson.pdf.