SUPPLEMENTARY MATERIALS: ANALYSING PATTERN FORMATION IN THE GRAY-SCOTT MODEL: AN XPPAUT TUTORIAL

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SM1. Analysis of Turing patterns. Turing showed that a slowly diffusing activator and a quickly diffusing inhibitor can generate a range of periodic patterns [SM2]. A reaction-diffusion system exhibits diffusion-driven instability, or Turing instability, if a homogeneous steady state is stable in the absence of diffusion, but unstable when diffusion is present. Here, we examine whether the Gray–Scott model can exhibit diffusion-driven instability to generate Turing patterns and, if so, where in (F, k)–space this occurs.

Derivation of the conditions that give rise to Turing instabilities is covered in full detail in [SM1]. We briefly summarise this procedure here. Let us firstly consider a general reaction–diffusion system of the form

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u + f(u, v), \tag{SM1.1a}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + g(u, v). \tag{SM1.1b}$$

Firstly, we want to obtain conditions for stability of a homogeneous steady state in the absence of diffusion. In the absence of diffusion, (SM1.1) reduces to

$$\frac{\partial u}{\partial t} = f(u, v), \qquad \frac{\partial v}{\partial t} = g(u, v). \tag{SM1.2}$$

The Jacobian for this system is given by

$$\mathbf{J} = \begin{bmatrix} f_u & f_v \\ g_u & g_v \end{bmatrix}. \tag{SM1.3}$$

For brevity, we assume that the derivatives f_u, f_v, g_u, and g_v are all to be evaluated at the steady state of interest, (u^*, v^*). To find the eigenvalues, we solve

$$|\mathbf{J} - \lambda \mathbf{I}| = \lambda^2 - \mathrm{tr}(\mathbf{J})\lambda + |\mathbf{J}| = 0, \tag{SM1.4}$$

with the quadratic formula to obtain

$$\lambda = \frac{1}{2}\left(\mathrm{tr}(\mathbf{J}) \pm \sqrt{\mathrm{tr}(\mathbf{J})^2 - 4|\mathbf{J}|}\right). \tag{SM1.5}$$

Linear stability requires both roots of (SM1.5) to satisfy $\mathrm{Re}(\lambda) < 0$. Therefore, we require $\mathrm{tr}(\mathbf{J}) < 0$, and also

$$\mathrm{tr}(\mathbf{J}) + \sqrt{\mathrm{tr}(\mathbf{J})^2 - 4|\mathbf{J}|} < 0. \tag{SM1.6}$$

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Since $\mathrm{tr}(\mathbf{J}) < 0$, (SM1.6) reduces to $|\mathbf{J}| > 0$. Therefore, the homogeneous steady state is stable in the absence of diffusion provided that both of the following conditions are satisfied:

$$\mathrm{tr}(\mathbf{J}) = f_u + g_v < 0, \tag{SM1.7a}$$

$$|\mathbf{J}| = f_u g_v - f_v g_u > 0. \tag{SM1.7b}$$

Next, we require conditions for a homogeneous steady state (u^*, v^*) to be unstable in the presence of diffusion. Linearising (SM1.1) by writing $u = u^* + \varepsilon\hat{u}$ and $v = v^* + \varepsilon\hat{v}$ (for some $\varepsilon \ll 1$), and neglecting terms of $\mathcal{O}\left(\varepsilon^2\right)$ provides

$$\mathbf{w}_t = \mathbf{J}\mathbf{w} + \mathbf{D}\nabla^2\mathbf{w} \tag{SM1.8}$$

where

$$\mathbf{w} = \begin{bmatrix} \hat{u} \\ \hat{v} \end{bmatrix}, \qquad \mathbf{D} = \begin{bmatrix} D_u & 0 \\ 0 & D_v \end{bmatrix}, \tag{SM1.9}$$

and $\mathbf{J}$ is the Jacobian matrix of (SM1.3). To allow analytical progress, we seek solutions that oscillate spatially and may grow or decay in amplitude over time, *i.e.* we let

$$\mathbf{w}(\mathbf{x}, t) = \sum_k c_k e^{\lambda t}\mathbf{W}_k(\mathbf{x}), \tag{SM1.10}$$

where $\mathbf{W}_k(\mathbf{x})$ is in Fourier series form, such that $\nabla^2\mathbf{W} = -k^2\mathbf{W}$. Substituting (SM1.10) in to (SM1.8), we obtain

$$\lambda\mathbf{w}(\mathbf{x}, t) = (\mathbf{J} - k^2\mathbf{D})\mathbf{w}(\mathbf{x}, t). \tag{SM1.11}$$

This has reduced to a manageable eigenvalue problem, with eigenvalue λ and matrix $\mathbf{J} - k^2\mathbf{D}$. We can obtain the characteristic polynomial in the usual way, by solving $|\lambda\mathbf{I} - \mathbf{J} + k^2\mathbf{D}| = 0$ to provide

$$\lambda^2 - p(k^2)\lambda + q(k^2) = 0, \tag{SM1.12}$$

where

$$p(k^2) = \mathrm{tr}(\mathbf{J}) - k^2(D_u + D_v), \tag{SM1.13a}$$

$$q(k^2) = D_u D_v k^4 - (D_v f_u + D_u g_v)\, k^2 + |\mathbf{J}|. \tag{SM1.13b}$$

Solving (SM1.12) using the quadratic formula, we determine the eigenvalues as

$$\lambda(k^2) = \frac{1}{2}\left(p(k^2) \pm \sqrt{p(k^2)^2 - 4q(k^2)}\right). \tag{SM1.14}$$

When $k = 0$, (SM1.14) is identical to (SM1.5). For the homogeneous steady state (u^*, v^*) to be unstable in the presence of diffusion, we require at least one eigenvalue to satisfy $\mathrm{Re}(\lambda) > 0$ for some $k \neq 0$.

From (SM1.7a), we have $\mathrm{tr}(\mathbf{J}) < 0$, and given that $D_u, D_v > 0$, it follows from (SM1.13a) that $p(k^2) < 0$ for all $k \neq 0$. Thus, requiring one eigenvalue to have positive real part equates to requiring

$$p(k^2) + \sqrt{p(k^2)^2 - 4q(k^2)} > 0, \tag{SM1.15}$$

or equivalently

$$\sqrt{p(k^2)^2 - 4q(k^2)} > |p(k^2)|. \tag{SM1.16}$$

We, thus, find that $\text{Re}(\lambda)$ can only be positive if $q(k^2) < 0$ for some $k \neq 0$.

From (SM1.7b), we have $|\mathbf{J}| > 0$, and given that $D_u, D_v > 0$, we have $q(k^2) < 0$ only if $D_v f_u + D_u g_v > 0$. However, in order to not contradict the requirement that $\text{tr}(\mathbf{J}) < 0$ from (SM1.7a), this is only possible for $D_u \neq D_v$. Therefore, our third condition for diffusion-driven instability is given by

$$D_v f_u + D_u g_v > 0, \qquad \frac{D_u}{D_v} \neq 1. \tag{SM1.17}$$

This condition is necessary but not sufficient for $\text{Re}(\lambda) > 0$. If $q(k^2) < 0$ for some $k \neq 0$, the minimum of $q(k^2)$ must be negative. We take $q(k^2)$ and differentiate with respect to k^2 to obtain

$$q'(k^2) = 2D_u D_v k^2 - (D_v f_u + D_u g_v). \tag{SM1.18}$$

Solving $q'(k^2) = 0$ yields

$$k^2 = \frac{(D_v f_u + D_u g_v)}{2D_u D_v}. \tag{SM1.19}$$

Substituting (SM1.19) into (SM1.13b) and performing some simplification yields

$$q_{min} = |\mathbf{J}| - \frac{(D_v f_u + D_u g_v)^2}{4D_u D_v}. \tag{SM1.20}$$

Requiring that $q_{min} < 0$ then provides the fourth and final condition for diffusion-driven instability, namely:

$$(D_v f_u + D_u g_v)^2 - 4D_u D_v |\mathbf{J}| > 0. \tag{SM1.21}$$

In summary, we have derived the following four conditions for diffusion-driven instability, or "Turing conditions":

$$\text{I.} \quad \text{tr}(\mathbf{J}) = f_u + g_v < 0, \tag{SM1.22a}$$

$$\text{II.} \quad |\mathbf{J}| = f_u g_v - f_v g_u > 0, \tag{SM1.22b}$$

$$\text{III.} \quad D_v f_u + D_u g_v > 0, \quad \frac{D_u}{D_v} \neq 1, \tag{SM1.22c}$$

$$\text{IV.} \quad (D_v f_u + D_u g_v)^2 - 4D_u D_v |\mathbf{J}| > 0. \tag{SM1.22d}$$

Now, let us return to the Gray–Scott model in particular, for which

$$f(u, v) = -uv^2 + F(1 - u), \tag{SM1.23a}$$

$$g(u, v) = uv^2 - (F + k)v. \tag{SM1.23b}$$

To investigate the scope for Turing patterns, we are interested in homogeneous steady states that are stable in the absence of diffusion. We have shown in Section 2 that there are two such steady states in this model: the red state $(1, 0)$ and the blue state (u^-, v^+). (We have already seen in Section 2 that the steady state at (u^+, v^-) is always unstable in the absence of diffusion, and so disregard this state here.)

Let us consider the red state initially. In Section 2, we showed that the fixed point at $(1, 0)$ is stable in the absence of diffusion for any choice of parameters F and k. However, (SM1.22c) requires that $D_v F + D_u(F + k) < 0$ for this steady state to be destabilised by diffusion. Since F, k, D_u and D_v are all positive parameters, this condition is never satisfied and we conclude that the red state does not exhibit diffusion-driven instability.

Now, consider the blue state at (u^-, v^+). In Section 2, we determined that this steady state is stable in the absence of diffusion anywhere in region II of Figure 1; this is equivalent to addressing the constraints of (SM1.22a) and (SM1.22b). To satisfy (SM1.22c), we require

$$(-{v^+}^2 - F) + D(2u^-v^+ - (F + k)) > 0, \tag{SM1.24}$$

where $D = D_u/D_v \neq 1$. Recalling that

$$(u^-, v^+) = \left(\frac{1}{2}\left(1 - \sqrt{X}\right), \frac{1}{2}\frac{F}{F + k}\left(1 + \sqrt{X}\right)\right), \tag{SM1.25}$$

where

$$X = 1 - \frac{4(F + k)^2}{F}, \tag{SM1.26}$$

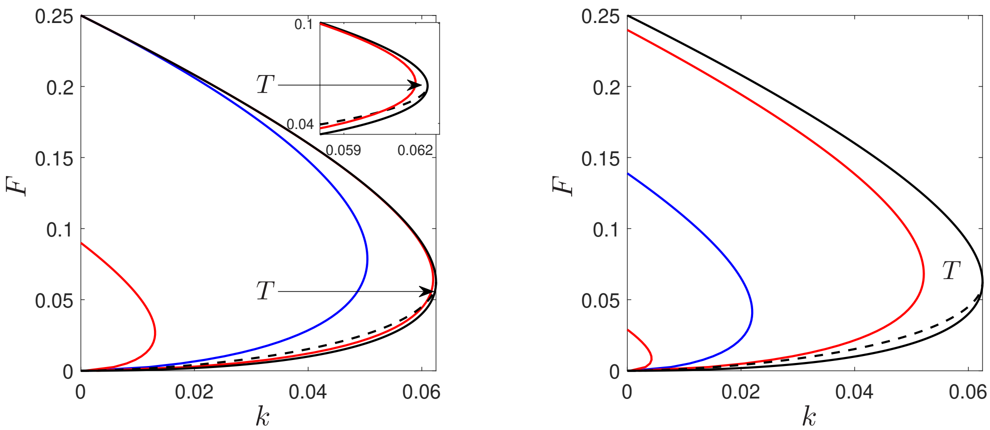
substitution of the the expressions for u^- and v^+ in to (SM1.24), and performing some rearrangement yields the following condition (which is equivalent to condition III of (SM1.22c)):

$$1 + \sqrt{1 - \frac{4(F + k)^2}{F}} - 2D\frac{(F + k)^3}{F^2} < 0. \tag{SM1.27}$$

Similarly, we substitute our expressions for f, g and (u^-, v^+) into (SM1.22d) and perform significant algebraic manipulation to construct condition IV for this steady state. Since the resulting expressions are lengthy and fairly complicated, we omit the details in full here, and instead calculate this condition numerically in Matlab.

In Figure SM1, we supplement the curves of Figure 1 with new curves representing our conditions for Turing instabilities, with condition III of (SM1.27) in blue and condition IV of (SM1.22d) in red. We illustrate this for both $D = 2$ and $D = 6$, here. Conditions I and II are satisfied in region II of Figure 1, while (in each panel of Figure SM1, condition III is satisfied to the right of the blue curve and condition IV is satisfied outside of the region bounded by the two red curves. We therefore obtain a region (labelled T the figure) in which Turing instabilites are permissible, giving rise to patterns. As Figure SM1 illustrates, the size of this region scales with the parameter D. For $D = 2$, the Turing space is very small, so the system exhibits diffusion-driven instability for a small range of parameters. As D is increased, the Turing space increases in size.

We provide Matlab code that can be used to solve the Gray–Scott model numerically on a two-dimensional domain (with periodic boundary conditions) online. This code utilises a five-point Laplacian to approximate the diffusion terms in (SM1.1) on a regular square mesh, and uses Euler's method to step solutions forward in time. Depending on our choices of the parameters F, k, D_u and D_v, and also on our choices of initial conditions, this code can be used to illustrate various patterns, including Turing patterns, the patterns of Figure 10, and others. (See the code online for



(a) $D = 2$.

(b) $D = 6$.

FIG. SM1. *Curves bounding the region of Turing patterns arising from the blue state for (a) $D = 2$ and (b) $D = 6$. The solid/dashed black lines are the saddle-node/Hopf bifurcations of Figure 1. The blue state is stable in the absence of diffusion within the solid black line and above the dashed black line (in region II of Figure 1).* (SM1.22c) *is satisfied everywhere to the right of the blue curve.* (SM1.22d) *is satisfied everywhere apart from between the two red lines. The region of parameter-space in which Turing patterns are permissible is labelled T in each figure; the size of this region scales with the parameter $D = D_u/D_v$.*

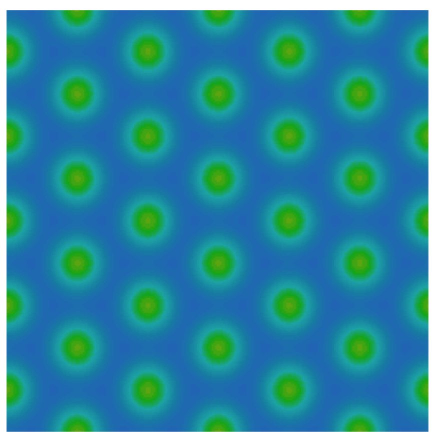


FIG. SM2. *A pattern comprising of a hexagonal array of spots that arises inside the Turing region for $D_u = 6 \times 10^{-5}$, $D_v = 1 \times 10^{-5}$ (i.e. for $D = 6$), $F = 0.195$ and $k = 0.02$.*

various pre-set configurations that can allow us to switch easily between these outcomes.) In particular, Figure SM2 illustrates the pattern that results from choosing a combination of parameters that lies within the region of Turing patterns illustrated in Figure SM1. In Figure SM2, we show the long-term pattern that arises for $F = 0.195$, $k = 0.02$, $D_u = 6 \times 10^{-5}$ and $D_v = 1 \times 10^{-5}$ (so that $D = 6$). Starting from an initial condition that perturbs the blue state, we see that the solution eventually converges to a hexagonal array of spots.

SM2. Exporting data from XPPAUT. Throughout this article, we have used Matlab to plot bifurcation diagrams generated by XPPAUT. This allows better control of presentation and formatting of the diagrams than is afforded by XPPAUT itself. In order to do this, we need to write the figure information to a data file in XPPAUT. There are two options for this, each with their own benefits.

In AUTO, Upon clicking `File`, the option `Write pts` will simply write the x and y values of the current diagram to a data file. In this file, the first two columns describe the x and y coordinates of the steady states plotted on the diagram. Additionally, the file includes a third column to account for additional y values that are obtained when plotting periodic orbits. (If the bifurcation diagram has no periodic orbits included, this will just be a duplicate of the previous column and can be discarded). Finally, the file will include three additional columns that contain arbitrary integer values that can be used to separate curves with different qualities (*e.g.* stable fixed points, unstable fixed points, stable periodic orbit, unstable periodic orbit *etc.*) that are plotted using different colours in XPPAUT. This data file can be imported directly into Matlab (as a Matlab table), and the data can be plotted accordingly. The task of associating the numerous rows of this data set with individual branches of the diagram is relatively manual and somewhat time-consuming, although there are some pre-existing codes available that can help to automate this process. See, for example, the function `SBplotxppaut` in Matlab's Systems Biology toolbox.

We note that the `Write pts` option only saves the information needed to recreate the current bifurcation diagram. For systems with many variables, only the plotted variable is stored. The other option is to write all of the information to a data file by clicking `File` (in the AUTO window), and then `All info`. This will save much more information about the bifurcation diagram, which isn't necessarily visible on the current plot. Since the saved data is more comprehensive, it is also more complicated to interpret manually and, for larger systems, can be too large for Matlab to handle. However, there are some great functions available online that can handle and plot this data; see, for example, https://uk.mathworks.com/matlabcentral/fileexchange/56819-mdepitta-plotbd.

REFERENCES

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