Supplementary Information for the *Journal of the Royal Society Interface* article "From One Pattern into Another: Analysis of Turing Patterns in Heterogeneous Domains via WKBJ" by A. L. Krause, V. Klika, T. E. Woolley, and E. A. Gaffney

S1. REDERIVATION OF TURING INSTABILITY WITH SPATIAL HOMOGENEITY.

The standard derivation of the Turing conditions in the homogeneous setting with Neumann boundary conditions considers the separable Fourier solution

$$\mathbf{w} \propto \exp(\lambda t)\cos(kx), \tag{S.1}$$

with wave number k, and finds the associated growth rate, λ. The conditions for a Turing instability then arise from the requirement that:

(i) there is stability when $k = 0$, indicating a stable steady state without diffusion,

(ii) a range of $k \neq 0$ generates an instability, at least providing k/π is a non-zero integer within this range.

In the heterogeneous case, the conditions associated with stability in the absence of diffusion are derived analogously to the homogeneous case. However, for instability, the Fourier solutions do not decouple and we seek an alternative approach. Proceeding, we firstly summarise the calculation of the homogeneous Turing conditions, where the fundamental equation arising from the substitution of (S.1) into (3) is given by

$$\det[\varepsilon^2 k^2 \mathbf{D} - \mathbf{J} + \lambda \mathbf{I}] = \det[\varepsilon^2 k^2 \mathbf{D} - \mathbf{J}_\lambda] = 0, \tag{S.2}$$

where we denote $\mathbf{J}_\lambda = \mathbf{J} - \lambda \mathbf{I}$. This condition is equivalent to

$$\det[-\mathbf{D}^{-1}\mathbf{J}_\lambda + \varepsilon^2 k^2 \mathbf{I}] = 0.$$

Hence, given ε and the wave number k, we can determine the growth rate λ. For a perturbation to grow we require values of k^2 and λ such that

$$\mathrm{Re}(\lambda) > 0, \quad \text{for} \quad k^2 = n^2\pi^2 > 0, \tag{S.3}$$

with n a non-zero integer, subject to Equation (S.2). Instead of following the normal approach where we vary k to ensure $\Re(\lambda) > 0$, we can instead vary λ to deduce conditions under which requiring k^2 to be real and positive implies the normal Turing conditions. The relationship between λ and k^2 is computed from the dispersion relation (S.2).

Non-real growth rates. Permissible values of k^2 are real and positive, or else we could not satisfy $k^2 = n^2\pi^2$ for an integer $n \neq 0$. Thus, we can exclude cases where $\varepsilon^2 k^2$ is not strictly real. We also neglect cases where $\mathrm{Re}(\lambda) < 0$ as we are only interested in instability. However we have

$$-\mathrm{tr}(\varepsilon^2 k^2 \mathbf{D} - \mathbf{J}) = [f_u + g_v - \varepsilon^2 k^2 (1+d)] < 0, \tag{S.4}$$

for permissible k^2, given that the homogeneous steady state is stable, so that $\mathrm{tr}(\mathbf{J}) = f_u + g_v < 0$. We also have from (S.2) that λ satisfies,

$$\lambda = -\mathrm{tr}(\varepsilon^2 k^2 \mathbf{D} - \mathbf{J}) \pm \sqrt{[\mathrm{tr}(\varepsilon^2 k^2 \mathbf{D} - \mathbf{J})]^2 - 4\det[\varepsilon^2 k^2 \mathbf{D} - \mathbf{J}]}. \tag{S.5}$$

Hence, if λ is non-real, its real part is negative as follows from (S.4)-(S.5). Thus, without loss of generality, we can consider real λ, as complex growth solutions with permitted wave numbers, if they exist, are stable.

Real growth rates. Recalling the notation $\mathbf{B}_0 = \mathbf{D}^{-1}\mathbf{J}$, the transition to instability occurs when $\lambda = 0$, whence

$$\varepsilon^2 k^2 = \frac{1}{2}\left[\mathrm{tr}(\mathbf{B}_0) \pm \sqrt{[\mathrm{tr}(\mathbf{B}_0)]^2 - 4\det(\mathbf{B}_0)}\right], \tag{S.6}$$

where the two roots $\varepsilon^2 k^2$ are the eigenvalues of $\mathbf{B}_0$. Therefore, to generate an inhomogeneous instability consistent with the stability of the zero mode (conditions (4)) we require

$$\mathrm{tr}(\mathbf{B}_0) - \sqrt{[\mathrm{tr}(\mathbf{B}_0)]^2 - 4\det(\mathbf{B}_0)} > 0. \tag{S.7}$$

There are two roots for $\varepsilon^2 k^2$ and *these are the eigenvalues of* $\mathbf{B}_0$. If both are negative, there is no permissible value of k^2, and thus there is no instability. If the smaller eigenvalue is negative and the larger is positive, then from the shape and behaviour of $\mathrm{Re}(\lambda)$ as a function of $\varepsilon^2 k^2$, one must have $\mathrm{Re}(\lambda) = \lambda > 0$ for $\varepsilon^2 k^2 = 0$. However, this possibility will be excluded as we require the mode associated with $k = 0$ to be stable. Thus we require that inequality (S.7) holds in order to generate an inhomogeneous instability consistent with the stability of the zero mode. In analogy to the standard derivation of the Turing condition, the requirement that k/π is a non-zero integer is only considered *a posteriori*. From the conditions for the stability of the zero mode, (4), we have that $\det(\mathbf{J}) > 0$, and hence $\det(\mathbf{D}^{-1}\mathbf{J}) > 0$. The remaining conditions for an inhomogeneous instability are then

$$\mathrm{tr}(\mathbf{D}^{-1}\mathbf{J}) > 0, \qquad [\mathrm{tr}(\mathbf{D}^{-1}\mathbf{J})]^2 - 4\det(\mathbf{D}^{-1}\mathbf{J}) > 0, \tag{S.8}$$

which are equivalent to the standard Turing conditions (5) given in Criterion (1).

S2. SINGULARITIES OF WKBJ MODES

Here we show properties of the solution near internal singular points in detail, denoting such a point as x_*. At any singular point, where $\mathbf{s}_*^T \mathbf{p}_* = 0$, the expression for Q_0, (10), becomes ill-defined, and hence we examine the structure of the solution near such a singular point.

With $\mathbf{J}_\lambda^*$ denoting $\mathbf{J}_\lambda(x_*)$ and similarly $\mathbf{B}_\lambda^* = \mathbf{B}_\lambda(x_*)$, we focus on the case when $\mathrm{tr}(\mathbf{J}^*) < 0$, $\det(\mathbf{J}^*) > 0$, $\mathrm{tr}(\mathbf{B}_\lambda^*) > 0$ which is the case of interest as this will be the boundary of $\mathcal{T}_\lambda$ (see Proposition 4). Further, the zero of $[\mathrm{tr}(\mathbf{B}_\lambda)]^2 - 4\det(\mathbf{B}_\lambda)$ is generically a simple one at $x = x_*$, as a non-simple zero would require mathematical fine-tuning in the model and parameter choices for smooth kinetic functions. Then for fixed $y \neq x_*$ with $\mathbf{s}_*^T \mathbf{p}_* \neq 0$ in (x_*, y), the integral

$$\exp\left[\int_x^y \frac{\mathbf{s}_*(\bar{x})^T \mathbf{p}_*'(\bar{x})}{\mathbf{s}_*(\bar{x})^T \mathbf{p}_*(\bar{x})} \mathrm{d}\bar{x}\right]$$

has a singularity which scales with $1/|x - x_*|^{1/4}$ as $x \to x_*$.

Proposition 9 *Let* λ *be a non-negative real growth rate. We assume* $\mathrm{tr}(\mathbf{J}^*) < 0$, $\det(\mathbf{J}^*) > 0$, *and* $\mathrm{tr}(\mathbf{B}_\lambda^*) > 0$ *with* $\mathbf{J}_\lambda^*$ *denoting* $\mathbf{J}_\lambda(x_*)$. *Additionally, we assume that the zero of* $[\mathrm{tr}(\mathbf{B}_\lambda)]^2 - 4\det(\mathbf{B}_\lambda))$ *is a simple one at* $x = x_*$. *Then with fixed* $y \neq x_*$ *the integral*

$$\exp\left[\int_x^y \frac{\mathbf{s}_*(\bar{x}) \cdot \mathbf{p}_*'(\bar{x})}{\mathbf{s}_*(\bar{x}) \cdot \mathbf{p}_*(\bar{x})} \mathrm{d}\bar{x}\right]$$

has a singularity which scales with $1/|x - x_*|^{1/4}$ *as* $x \to x_*$.

Proof. By (19) we have

$$\mu_\lambda^\pm(x_*) = \frac{1}{2}\mathrm{tr}(\mathbf{B}_\lambda^*),$$

which is a double root at $x = x_*$, so we have,

$$[-\mu_\lambda^\pm(x_*)\mathbf{I} + \mathbf{D}^{-1}\mathbf{J}_\lambda] = \begin{pmatrix} f_u - \lambda - \mu_\lambda^\pm & f_v \\ \dfrac{g_u}{d} & \dfrac{g_v - \lambda}{d} - \mu_\lambda^\pm \end{pmatrix}, \quad (f_u - \lambda - \mu_\lambda^\pm)\left(\frac{g_v - \lambda}{d} - \mu_\lambda^\pm\right) - \frac{1}{d} f_v g_u = 0. \tag{S.9}$$

With sign choices that are without loss of generality, we compute

$$\mathbf{p}_*(x) = \frac{1}{R_p}\begin{pmatrix} -f_v \\ f_u - \lambda - \mu_\lambda^\pm \end{pmatrix}, \qquad R_p = \left(f_v^2 + |f_u - \lambda - \mu_\lambda^\pm|^2\right)^{1/2},$$

with

$$\mathbf{s}_*(x) = \frac{1}{R_s}\left(-g_u/d, f_u - \lambda - \mu_\lambda^\pm\right), \qquad R_s = \left(\left(\frac{g_u}{d}\right)^2 + |f_u - \lambda - \mu_\lambda^\pm|^2\right)^{1/2}.$$

We will need $R_p \sim O(1)$ near $x = x_*$, and so must show that $R_p(x_*) \neq 0$. We proceed by contradiction and assume that $R_p = 0$ at $x = x_*$. Then $f_u - \lambda - \mu_\lambda^\pm = 0 = f_v$. So therefore $f_u > \lambda > 0$, but we have $\det(\mathbf{J}^*) = f_u g_v > 0$ and $\mathrm{tr}(\mathbf{J}^*) = f_u + g_v < 0$, which cannot be simultaneously satisfied, and hence we must have $R_p \neq 0$ at $x = x_*$. An analogous proof also shows that $R_s \neq 0$ at $x = x_*$.

Letting $x = x_* + X$ with $|X| \ll 1$, and defining

$$\alpha_\lambda = \frac{\partial}{\partial x}\left([\mathrm{tr}(\mathbf{B}_\lambda)]^2 - 4\det(\mathbf{B}_\lambda)\right)\Big|_{x=x_*},$$

we have from equation (19) that near $x = x_*$

$$\mu_\lambda^\pm(x) := \frac{1}{2}\left\{\begin{array}{ll} \left[\mathrm{tr}(\mathbf{B}_\lambda^*) \pm |\alpha_\lambda X|^{1/2} + O(X)\right] & \alpha_\lambda X > 0 \\ \left[\mathrm{tr}(\mathbf{B}_\lambda^*) \pm i|\alpha_\lambda X|^{1/2} + O(X)\right] & \alpha_\lambda X < 0 \end{array}\right\} := \mu_\lambda^{0*} + \frac{1}{2}\left\{\begin{array}{ll} \pm|\alpha_\lambda X|^{1/2} + O(X) & \alpha_\lambda X > 0 \\ \pm i|\alpha_\lambda X|^{1/2} + O(X) & \alpha_\lambda X < 0 \end{array}\right\}, \tag{S.10}$$

where $\mu_\lambda^{0*} = \mathrm{tr}(\mathbf{B}_\lambda^*)$ is constant in X. We do not consider the degenerate case of $\alpha_\lambda = 0$ as this corresponds to a non-simple root of $\det([-\mu_\lambda^\pm(x)\mathbf{I} + \mathbf{D}^{-1}\mathbf{J}_\lambda])$ at $x = x_*$. From this expansion, we have (denoting derivatives with respect to X as $' \equiv \partial_X$)

$$(\mu_\lambda'^\pm)(x) = \frac{1}{4}\left\{\begin{array}{ll} \pm\left|\dfrac{\alpha_\lambda}{X}\right|^{1/2} + O(1) & \alpha_\lambda X > 0 \\ \pm i\left|\dfrac{\alpha_\lambda}{X}\right|^{1/2} + O(1) & \alpha_\lambda X < 0 \end{array}\right\}. \tag{S.11}$$

Specialising in the first instance to the case $\alpha_\lambda X > 0$, and on noting $f_u = f_u^* + O(|X|)$, $f_v = f_v^* + O(|X|)$ near $x = x_*$, while $R_p^* = R_p(x_*) \sim O(1)$, $R_s^* = R_s(x_*) \sim O(1)$, the contraction of $\mathbf{s}_*(x)$ and $\mathbf{p}_*(x)$ yields

$$\begin{aligned}
\mathbf{s}_*(x)\cdot\mathbf{p}_*(x) &= \frac{1}{R_p R_s}\left[\frac{1}{d}f_v g_u + (f_u - \lambda - \mu_\lambda)^2\right] \\
&= \mathbf{s}_*(x_*)\cdot\mathbf{p}_*(x_*) \mp \frac{1}{R_p^* R_s^*(1 + O(|X|^{1/2}))}\left[(f_u^* - \lambda - \mu_\lambda^{0*})|\alpha_\lambda X|^{1/2} + O(|X|)\right] \\
&= \mp\frac{1}{R_p^* R_s^*}(f_u^* - \lambda - \mu_\lambda^{0*})|\alpha_\lambda X|^{1/2} + O(|X|), \quad \text{as } X \to 0.
\end{aligned}$$

Further, on differentiating $\mathbf{p}_*(x)$, one finds

$$\mathbf{p}_*'(x) = \frac{1}{R_p}\left(\begin{array}{c} -f_v \\ f_u - \lambda - \mu_\lambda \end{array}\right)' - \frac{R_p'}{R_p^2}\left(\begin{array}{c} -f_v \\ f_u - \lambda - \mu_\lambda \end{array}\right) = \frac{1}{4R_p^*}\left(\begin{array}{c} O(1) \\ \mp\left|\dfrac{\alpha_\lambda}{X}\right|^{1/2} \end{array}\right) + O(1) - \frac{R_p'}{R_p}\mathbf{p}_*(x).$$

Contracting with $\mathbf{s}_*(x)$ yields

$$\mathbf{s}_*(x)\cdot\mathbf{p}_*'(x) = \mp\frac{1}{4R_p^* R_s^*}\left[f_u^* - \lambda - \mu_\lambda^{0*}\right]\left|\frac{\alpha_\lambda}{X}\right|^{1/2} + O(1) - \frac{R_p'}{R_p}\mathbf{s}_*(x)\cdot\mathbf{p}_*(x) = \mp\frac{1}{4R_p^* R_s^*}\left[f_u^* - \lambda - \mu_\lambda^{0*}\right]\left|\frac{\alpha_\lambda}{X}\right|^{1/2} + O(1),$$

on noting that

$$R_p' \sim O\left(\left|\frac{\alpha_\lambda}{X}\right|^{1/2}\right), \quad \mathbf{s}_*(x)\cdot\mathbf{p}_*(x) \sim O\left(|X|^{1/2}\right), \quad \text{as } X \to 0.$$

Hence

$$\frac{\mathbf{s}_*(x)\cdot\mathbf{p}'_*(x)}{\mathbf{s}_*(x)\cdot\mathbf{p}_*(x)} = \frac{1}{4|X|}\left(1+O(|X^{1/2}|)\right), \tag{S.12}$$

and the above calculations hold for arbitrary $\alpha_\lambda \neq 0$ and thus equation (S.12) also holds for $\alpha_\lambda X < 0$. In turn, we have for $x = x_* + X$, $X > 0$,

$$\frac{Q_0(x_*+X)}{Q_0(1)} \propto \exp\left[-\int_1^{x_*+X}\frac{\mathbf{s}_*(\bar{x})\cdot\mathbf{p}'_*(\bar{x})}{\mathbf{s}_*(\bar{x})\cdot\mathbf{p}_*(\bar{x})}\mathrm{d}\bar{x}\right] = \exp\left[\int_{x_*+X}^{1}\frac{1}{4(\bar{x}-x_*)}+O\left(\frac{1}{(\bar{x}-x_*)^{1/2}}\right)\mathrm{d}\bar{x}\right] \sim O\left(\frac{1}{|X|^{1/4}}\right),$$

and the same scaling holds for $X < 0$. ■

On approaching such a singular point x_*, solutions and their derivatives become unbounded and the asymptotic assumptions inherent in the WKBJ approximation (that the diffusion term is subleading), breaks down. In contrast, the second derivative of such solutions near $x \approx x_*$ will scale with $1/|x-x_*|^{9/4}$, and hence the transport term is no longer asymptotically small when $|x-x_*| \sim \varepsilon^{8/9}$. Hence boundary layers are present around x_*. However, the interior boundary layer problem is not tractable analytically, and thus we only consider the outer WKBJ solutions. Nonetheless, we require boundedness of the outer solutions on approaching the boundary layer, otherwise such solutions will be arbitrarily large for sufficiently small ε. In turn the outer region is valid for $|x-x_*| \sim \varepsilon^{4/9} \gg \varepsilon^{8/9}$, where the WKBJ solution scales with $1/|x-x_*|^{1/4} \sim 1/\varepsilon^{1/9} \to \infty$ as $\varepsilon \to 0$. Solution boundedness requires the expression in (11) to take the form of a sin function near the singular point x_*, and a cos function is used at a zero-flux boundary.

S3. RELATIONSHIP BETWEEN $n^\pm$ AND λ AND THE SUPPORT OF NON-TRIVIAL WKBJ MODES

Here we show that λ decreases with n^+ in the positive branch of WKBJ solutions, and outline how the negative branch behaves.

Proposition 10 *The value of the non-negative growth rate λ decreases with n^+ for the positive branch of WKBJ solutions.*

Proof. We proceed by differentiating the fundamental constraint (16) with respect to $n^\pm$ to find

$$\lambda'(n^\pm)\left[b'(\lambda)\sqrt{\mu_\lambda^\pm(b(\lambda))}-a'(\lambda)\sqrt{\mu_\lambda^\pm(a(\lambda))}+\int_{a(\lambda)}^{b(\lambda)}\frac{\partial_\lambda(\mu_\lambda^\pm)(\bar{x})}{2\sqrt{\mu_\lambda^\pm(\bar{x})}}\mathrm{d}\bar{x}\right] = \pi\varepsilon > 0. \tag{S.13}$$

By Proposition 8 we have that $a'(\lambda) \geq 0$ and $b'(\lambda) \leq 0$, which implies that the first two terms of (S.13) are together negative and we must only check the sign of the third term. For the positive branch, this term is negative by the proof of Proposition 5, as $\partial_\lambda \mu_\lambda^+ < 0$, hence, for this branch we must have $\lambda'(n^+) < 0$. ■

Any non-trivial WKBJ solution has a support (in space) demarcated by singular points $x_*(\lambda(n^\pm)) =: x_*(\lambda)$ or the domain boundaries. Therefore the support of the n^+-th mode also decreases (or remains the same) as n^+ is increased, due to the monotonicity of $\mathcal{T}_\lambda$. We can conclude that $\mathcal{T}_{\lambda(n+)}$ shrinks with increasing n^+, and that the largest permissible n^+ will correspond to the smallest value of λ and the largest spatial support, whereas the smallest n^+ will have the smallest support, but largest growth rate.

For the negative branch n^-, the calculation in the proof of Proposition 10 reveals that a competition between two terms of different signs takes place, and the overall picture is more complicated. First, note that if there is no singular point within the domain $[0,1]$ for a range of λ, then the first two boundary terms of (S.13) vanish and the last term was shown to be positive via the proof in Proposition 5 for μ_λ^-. Hence, in this scenario, λ would increase with increasing n^-. In the case when there is an internal singular point, we know that $\mathcal{T}_\lambda$ decreases with increasing λ. Additionally, near the maximal permissible λ, the support of the fastest growing mode is very small and becomes a strict subset of $[0,1]$. Further, for such maximal admissible λ, both $n^\pm = 1$ as $\mu_\lambda^\pm(x)$ is a continuous function in λ and in $x \in [a,b]$ including the boundaries, while we know that $\mathcal{T}_\lambda$ is monotonic in λ. Hence, the left hand side of equation (27) is arbitrarily small and as a result $n^\pm = 1$ for the largest admissible λ. Therefore, close to this maximal value, λ has to decrease with n^-. Finally, as all the terms determining the sign of $\lambda'(n^-)$ have a fixed sign, we know that there is at most one extremum of $\lambda(n^-)$, which then completes the picture for the negative branch.

In Fig. S1 we show the support of each discrete mode alongside its corresponding growth rate for both solution branches. We highlight regions corresponding to the four modes of each branch given in Fig. 6. We note in particular that the fastest

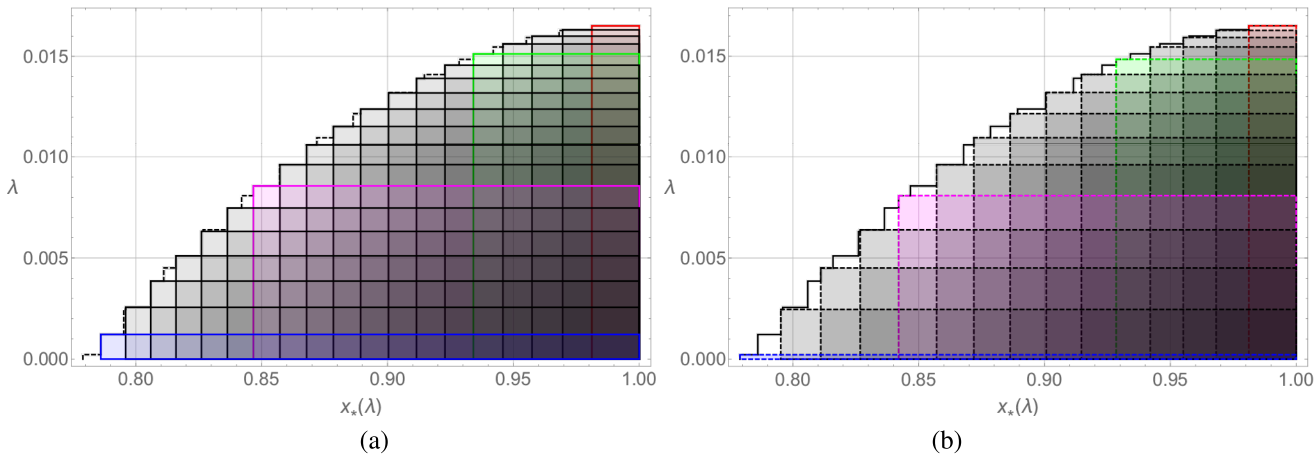

FIG. S1: The "structure" of a patterned state linear analysis showing the intervals where a given WKBJ solution from the positive branch ((a), solid lines) and from the negative branch ((b), dashed lines) will dominate. The discreteness of the steps is highlighted together with the value of growth rate λ. For each mode we plot an opaque rectangle with the horizontal side being the support of the mode,i.e. the interval $(x_*(\lambda(n^{\pm})),1)$, while the vertical side is the value of the growth rate for a given mode $\lambda(n^{\pm})$. Note that the highlighted rectangles in colors correspond to the modes depicted in Fig 6. Hence, there are subintervals where many modes exist. The envelope of the largest λ values then forms then the topmost black line at the boundary, which we conjecture to have a relation to the amplitude envelope of emerging patterned solutions.

growing mode in any given spatial region is the mode which is highest in any given region in Fig. S1, and hence this changes as each subsequent mode becomes permissible (i.e. moving left to right each new mode has a larger value of λ). Hence we conjecture that if all modes are approximately excited by the same amount, then the envelope of unstable modes should scale with the fastest growing mode locally, which is qualitatively observed in Fig. 4. Additionally, in the homogeneous setting, close to a supercritical bifurcation any patterned state should have an amplitude which scales with λ raised to a power, and hence this provides an intuition for the final small-amplitude patterns observed in Figs. 2-3, as again the envelope of the oscillations should scale with λ. However, we do not formally deduce a relationship between the envelope of the final patterned state with λ, and instead leave this as future work.