Mesa-type structures and their stability in the Brusselator

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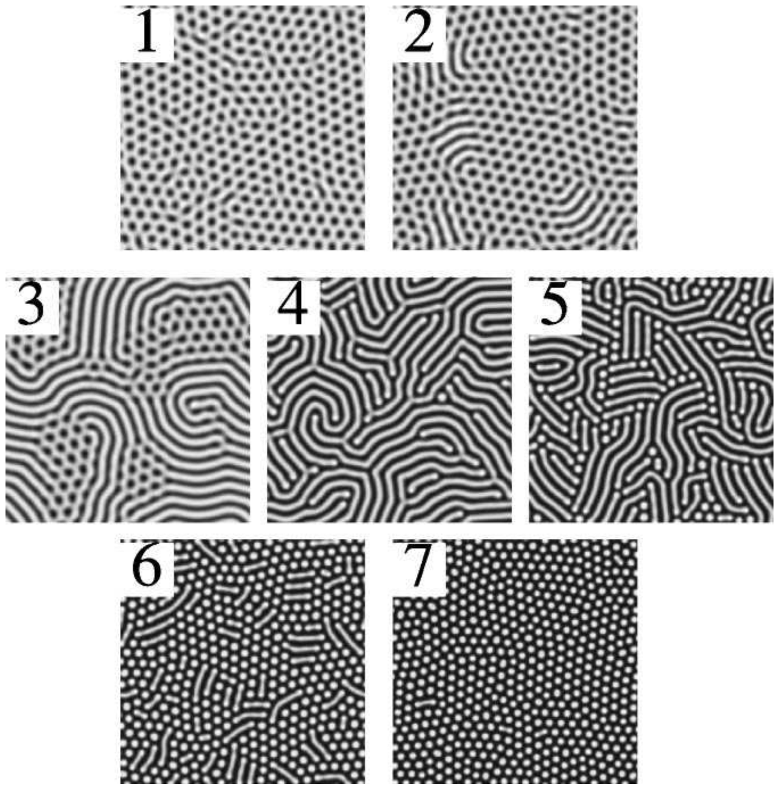
Brief history

- 1952: Turing instability
- 1968: Prigogine, Lefever, propose the Brusselator
- 1970's: Nicolis, Prigogine, Erneux, Turing patterns in the Brusselator
- 1980-2000's: Spots, stripes, hexagonal patterns, oscillatory instabilties, spatio-temporal chaos: Erneux, Reiss, De Wit, Brockmans, Dewel, Kidachi, Pena, Perez-Garcia

Some examples of patterns in 2-D:



Reference: B. Peña and C. Pérez-García, *Stability of Turing patterns in the Brusselator model*, Phys. Rev. E. Vol. 64(5), 2001.

The Brusselator model

Rate equations:

$$A \xrightarrow{\varepsilon} X, \quad B+X \to Y+D, \quad 2X+Y \to 3X, \quad X \xrightarrow{\varepsilon} E.$$

After rescaling, we get a PDE system:

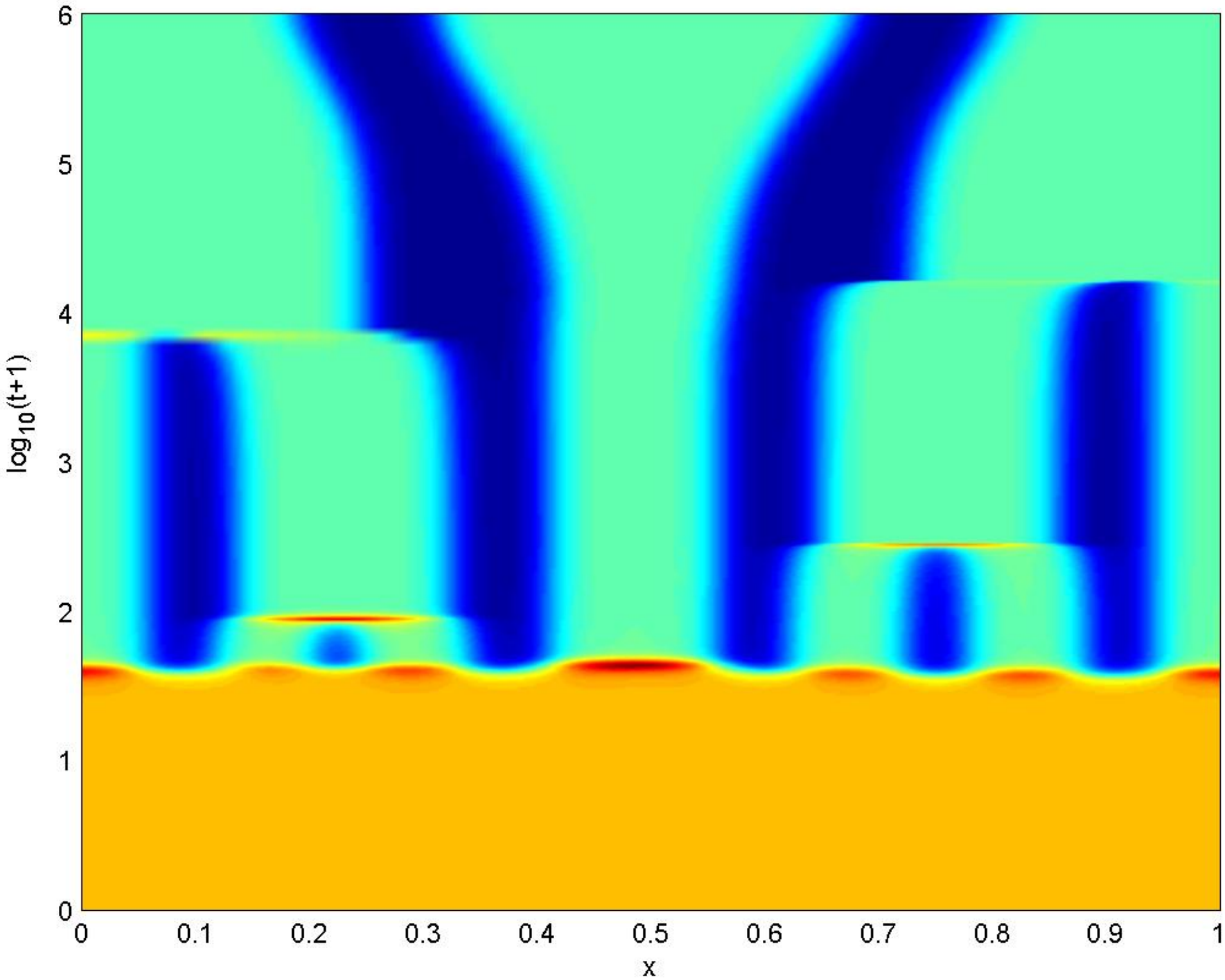
$$\begin{aligned} v_t &= \varepsilon D v_{xx} + Bu - u^2 v, \\ \tau u_t &= \varepsilon D u_{xx} + \varepsilon A + u^2 v - (B + \varepsilon)\, u \end{aligned}$$

on the interval $[0, 1]$ with Neumann boundary conditions.

We assume:

$$\varepsilon D \ll 1; \quad D \gg 1.$$

Coarsening process



$$A = 1, B = 8,\ \varepsilon = 10^{-4},\ D = 10,\ \tau = 10.$$

Steady state

$$0 = \varepsilon D v_{xx} + Bu - u^2 v,$$
$$0 = \varepsilon D u_{xx} + \varepsilon A + u^2 v - (B + \varepsilon)\, u$$

Let $w = v + u$; then

$$0 = \delta^2 v_{xx} + B\,(w - v) - (w - v)^2\, v,$$
$$0 = D w_{xx} - w + v + A$$

where $\delta^2 = \varepsilon D \ll 0$ and $D \gg 1$. Therefore

$$w \sim w_0$$

is constant to first order; and $\delta^2 v_{xx} = \text{Cubic}(v)$. The **Maxwell line** condition then implies:

$$B = \frac{2}{9} w_0^2.$$

Away from interfaces, $v \sim w_0$ or $v \sim w_0/3$. Near the interface x_0,

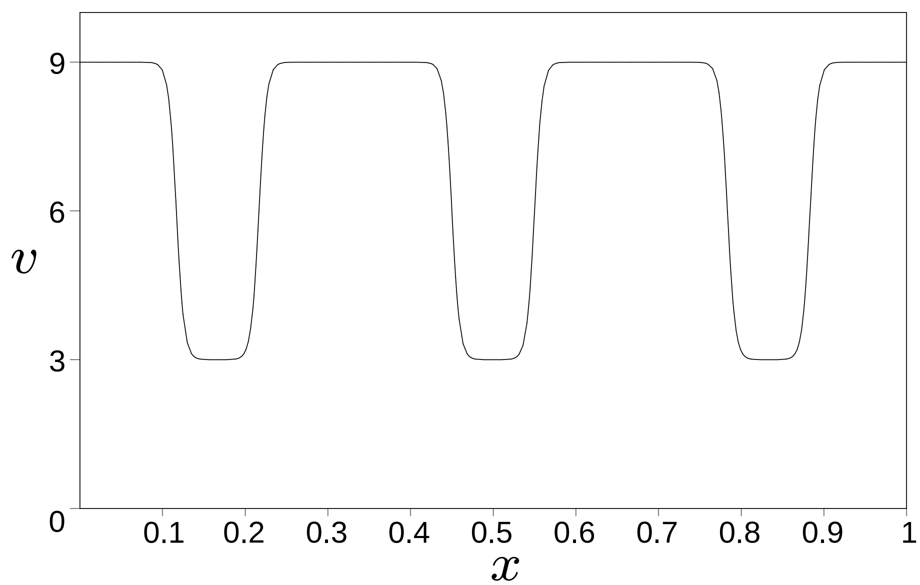
$$v \sim w_0 \frac{2}{3} \pm w_0 \frac{1}{3} \tanh\left(\frac{w_0}{3} \frac{(x - x_0)}{\sqrt{2\varepsilon D}}\right)$$

Suppose $v \sim w_0/3$ on $[0, l]$ and $v \sim w_0$ on $[l, 1]$. Using solvability condition we obtain,

$$w_0 - A = \int_0^1 v = l w_0/3 + (1 - l) w_0$$

and so

$$l = \frac{A}{\sqrt{2B}}.$$



An example of a three-mesa equilibrium state for v. Here, $K = 3$, $A = 2$, $B = 18$, $\varepsilon D = 0.02^2$.

Stability of K mesas

Theorem 1 *Consider a K mesa equilibrium state. Suppose that*

$$1 \ll DK^2 \ll O\left(\frac{1}{\varepsilon \ln^2 \varepsilon}\right) \qquad \textit{and} \quad O(\tau - 1) \gg 0.$$

Such solution is stable when $\tau - 1 \gg 0$ and unstable when $\tau - 1 \ll 0$. There are $2K$ small eigenvalues of order $O(\varepsilon)$; all other eigenvalues are negative and have order $\leq O(D\varepsilon)$. The smallest $2K$ eigenvalues are given by

$$\lambda_{j\pm} \sim \frac{-1 \pm \sqrt{1 - 2K^2 dl \left[1 - \cos\left(\frac{\pi j}{K}\right)\right]}}{2(\tau - 1)} \varepsilon,$$
$$j = 1 \ldots K - 1;$$
$$\lambda_- \sim \frac{-Kl}{\tau - 1}\varepsilon, \qquad \lambda_+ = \frac{-1}{\tau - 1}\varepsilon.$$

and are all negative when $\tau > 1$, and positive when $\tau < 1$. The transition from stability to instability occurs via a Hopf bifurcation as τ is decreased past τ_h where to leading order, $\tau_h \sim 1$.

Theorem 2 *Suppose that*

$$\tau > 1$$

and let

$$D_K = \frac{1}{K^2} D_1 \quad \textit{where}$$

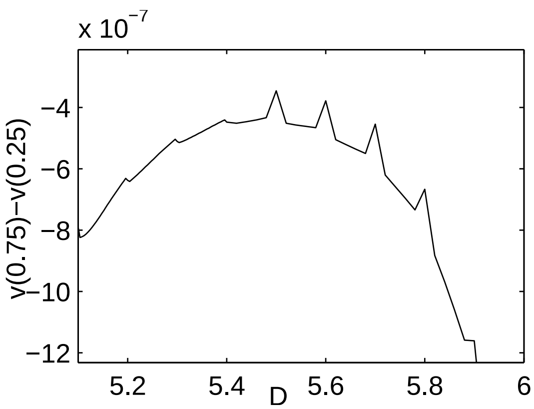
$$D_1 \sim \begin{cases} \dfrac{A^2}{2\varepsilon \ln^2\left(\frac{12\sqrt{2}AB^{3/2}}{\varepsilon\left(\sqrt{2B}-A\right)^2}\right)}, & 2A^2 < B \\ \dfrac{\left(\sqrt{2B}-A\right)^2}{2\varepsilon \ln^2\left(\frac{12\sqrt{2}}{\varepsilon A}B^{3/2}\right)}, & 2A^2 > B \end{cases} + l.s.t.$$

Here, l.s.t. denotes logarithmically small terms. Then a K mesa symmetric equilibria with $K \geq 2$ is stable if $D < D_K$ and is unstable otherwise. Moreover, a single-mesa equilibria $K = 1$ is always stable.

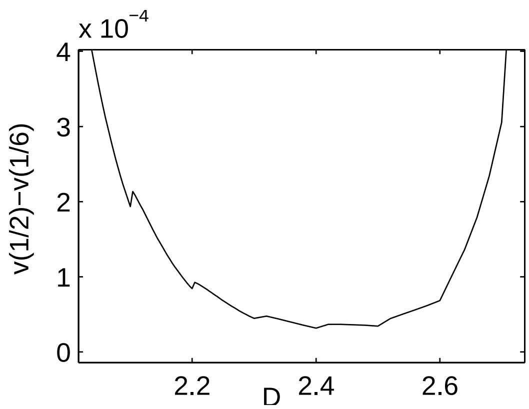
Example of Theorem 2

Take $\varepsilon = 0.001$, $A = 2$, $B = 18, \tau = 3$; then

$$D_1 = 21.16, D_2 = 5.3, \quad D_3 = 2.35.$$



(a)



(b)

(a) $K = 3$, $D = 5 + 0.1\text{floor}(t/2500)$. Change of stability when $D \sim 5.5$.

(b) $K = 2$, $D = 1.9{+}0.1\text{floor}(t/2500)$. Change of stability when $D \sim 2.45$.

The condition

$$DK^2 = O\left(\frac{1}{\varepsilon \ln^2 \varepsilon}\right)$$

can be rewritten as

$$D = O\left(\delta^2 \exp\left\{\frac{1}{K\delta}\right\}\right)$$

where $\delta = \sqrt{\varepsilon D}$ is the characteristic width of the interface. Thus the instability threhold occurs when D is exponentially large compared to $\frac{1}{K\delta}$. In this case the exponentially small interactions in the tail of v become of the same order as other terms in the calculation and is the cause of the instability.

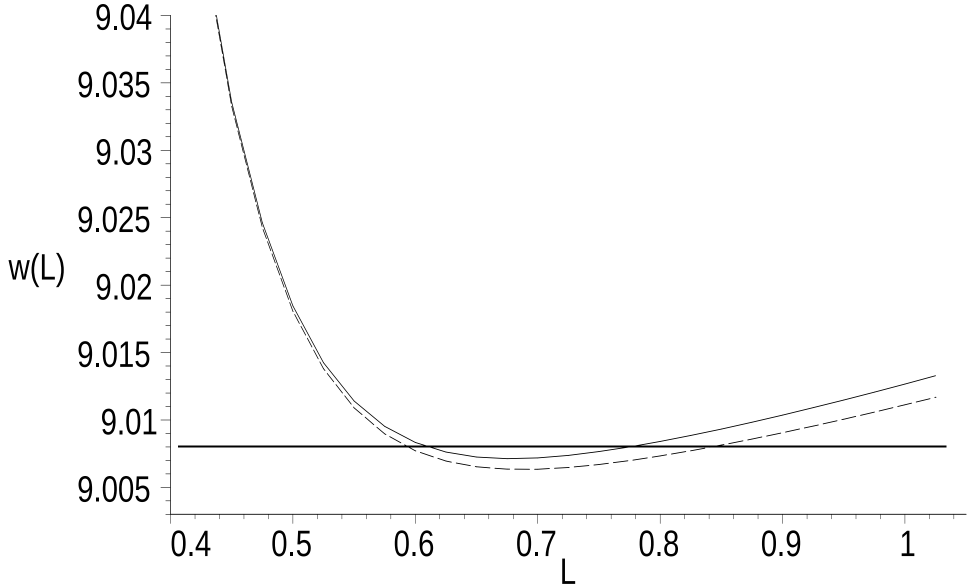
Asymmetric patterns

Consider a single symmetric mesa solution on domain $[0, L]$. Second order computation yields,

$$w(L) \sim 3\sqrt{B/2} + \frac{1}{D}\frac{A}{16B}L^2\left(\sqrt{2B} - A\right)^2 \\ + 3\sqrt{2B}\left(\exp\left\{-\frac{LA}{\sqrt{2\varepsilon D}}\right\} + \exp\left\{-\frac{L}{\sqrt{2\varepsilon D}}\left(\sqrt{2B} - A\right)\right\}\right)$$

The minimum of the curve $L \to w(L)$ occurs when $D/L^2 = O\left(\frac{1}{\varepsilon \ln^2 \varepsilon}\right)$. At that point an asymmetric solution bifurcates from the symmetric branch. This point coincides with the instability threshold after taking $L = 1/K$.

Example: $A = 2$, $B = 18$, $\varepsilon = 0.001$ and $D = 10$.



Asymmetric solution is obtained by gluing together two solutions on different intervals but with the same height. Here a two-mesa asymmetric solution is constructed on interval of length $\sim 0.6 + 0.8$.

Comparison with Turing instability

The instability of Theorem 2 occurs when

$$K = K^* = O\left(\frac{1}{\delta \ln \frac{1}{\varepsilon}}\right)$$

where $\delta = \sqrt{D\varepsilon}$ is the charactersitic interface width.

When $B > A^2$, the modes in the Turing instability band all have the order

$$k = O\left(\frac{1}{\delta}\right).$$

It is then clear that $k \gg K$ by a logarithmically large amount. Therefore coarsening is expected if initial condition is a homogeneous steady state.

When $B < A^2$, the homogeneous steady state is stable with respect to Turing. But stable mesa solutions also occur!

Breather-type instability

Lemma 1 *Suppose that*

$$1 \ll DK^2 \ll O\left(\frac{1}{\varepsilon}\ln^2\varepsilon\right).$$

The eigenvalues of such equilibrium state are given implicitly by

$$\lambda \sim 2\sqrt{B\frac{\varepsilon}{D}}\left(ldK - \frac{2}{\sigma}\frac{(\tau-1)\lambda+\varepsilon}{\varepsilon}\right)$$

where σ is one of

$$\sigma_{j\pm} = c \pm \sqrt{a^2+b^2+2ab\cos\left(\frac{\pi j}{K}\right)}, \quad j = 1\ldots K-1$$

$$\sigma_{\pm} = c + a \pm b$$

where

$$a = \frac{-\mu_d}{\sinh(\mu_d d)}, \qquad b = \frac{-\mu_l}{\sinh(\mu_l l)},$$

$$c = \mu_d \coth(\mu_d d) + \mu_l \coth(\mu_l l),$$

$$\mu_l \equiv \frac{\sqrt{2\varepsilon+\lambda(2\tau-1)}}{\delta}, \qquad \mu_d \equiv \frac{\sqrt{\lambda}}{\delta}.$$

Theorem 3 *Suppose that*

$$\sqrt{\frac{B}{\varepsilon D}} \ll DK^2 \ll O\left(\frac{1}{\varepsilon \ln^2 \varepsilon}\right).$$

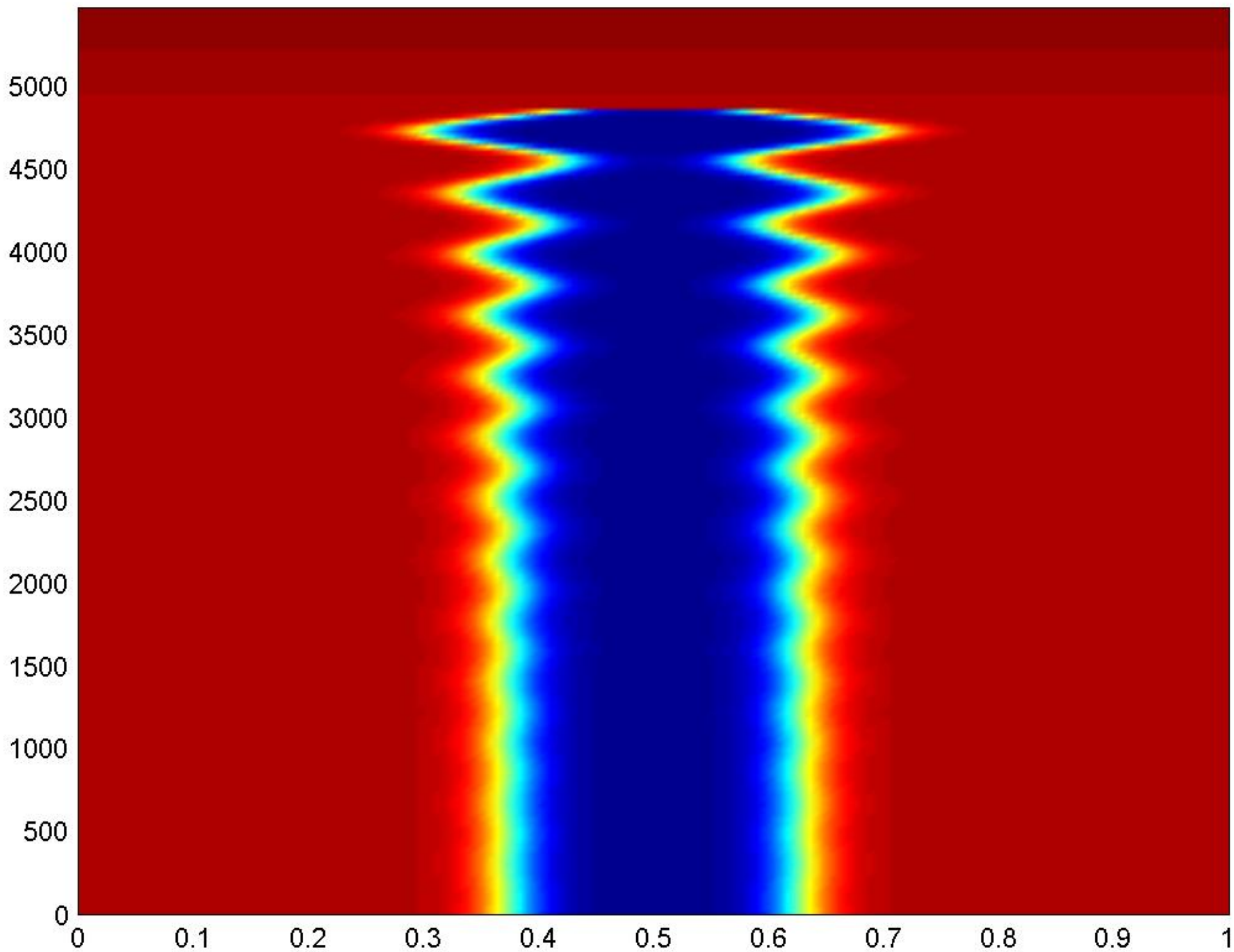
Let

$$\tau_{h_+} = 1 + \frac{1}{4D}\left(ld - \frac{K}{3}\left(d^3 + l^3\right)\right)$$

Then a K-mesa solution undergoes a Hopf bifurcation when $\tau = \tau_{h_+}$. *It is stable when* $\tau > \tau_{h_+}$ *and unstable otherwise. When* $\tau = \tau_{h_+}$, *the corresponding eigenvalue has value*

$$\lambda_+ \sim i\sqrt{8K}\left(\varepsilon^3 DB\right)^{1/4}$$

Example



From Theorem 3, $\lambda_+ \sim 0.0168$ so that one period is $P = \frac{2\pi}{\lambda_+} \sim 373.5$. This agrees with an estimate $P = 400$ from the figure.

Open question 1

Study the limit of small mesa width $l \to 0$.

- A single mesa admits two small eigenvalues, $\lambda_\pm$. λ_+ corresponds to even perturbations, causing the breather instability. λ_- corresponds to an odd perturbation which can lead to oscillatory travelling mesa. However numerically only λ_+ is observed.

- For Gray-Scott model, oscillatory travelling instability was also observed in the spike regime.

- Does Brusselator also admit oscillatory travelling instability in the limit where the width of the mesa $l \to 0$?

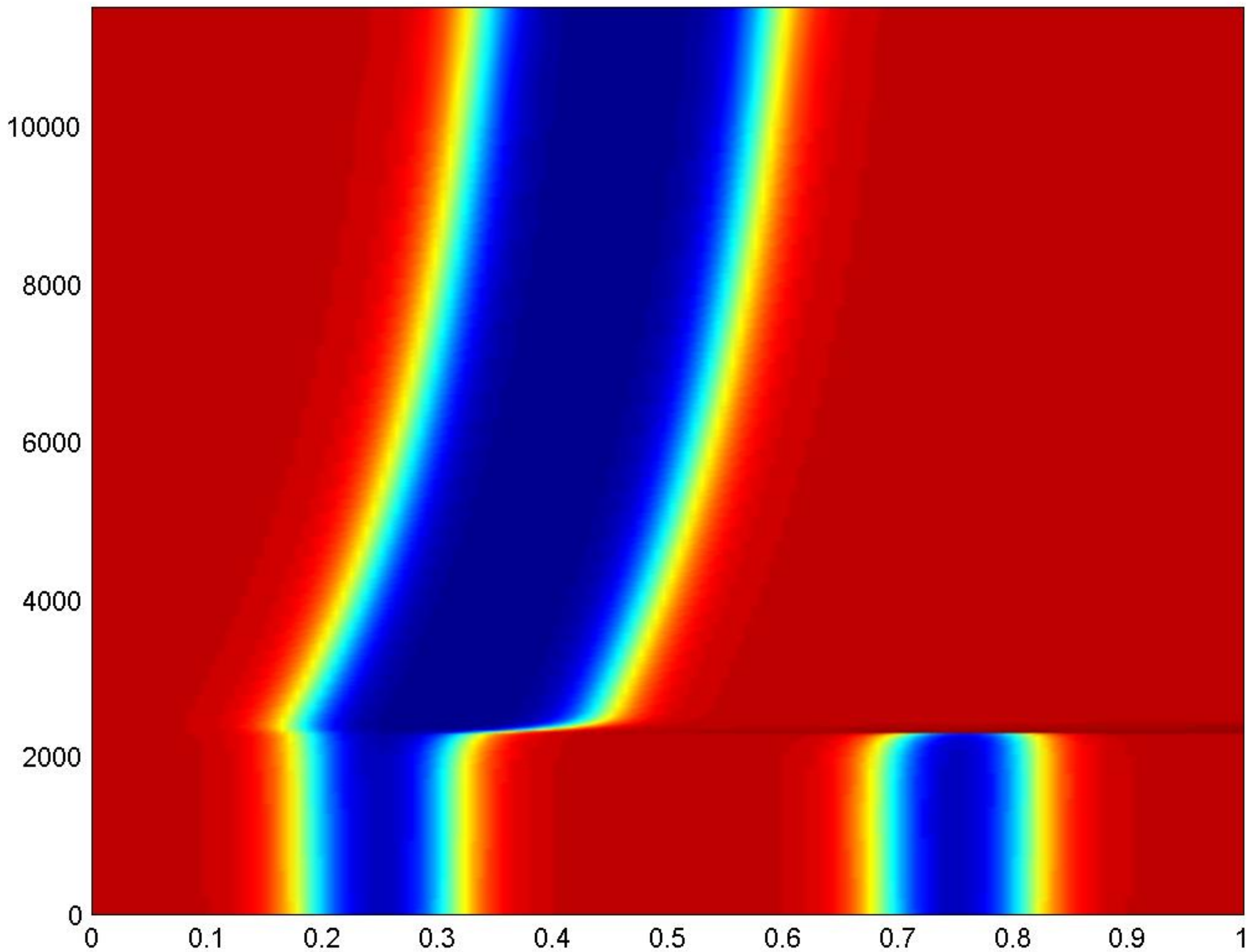
Open question 2

Does there exist a regime where both the homogeneous steady state is unstable with respect to Turing and mesa structure is unstable with respect to breather instability? (if yes, then we expect spatio-temporal chaos).

If $O(\sqrt{\frac{B}{\varepsilon D}}) \ll D \ll O\left(\frac{1}{\varepsilon \ln^2 \varepsilon}\right)$ then the answer is no.

Open question 3

Describe the slow dynamics of the mesas. There



- slow mass exchange ($t \sim 0 - 2000$)
- slow motion ($t > 2200$)

Comparison to other bistable systems

- Brusselator: Has an asymptotic "mass conservation" law. Coarsening process terminates when $K = K^* \gg 1$. Algebraically slow dynamics?

- Cahn-Hilliard: Has a variational structure, exact mass conservation. Coarsening proceeds until only one interface is left. Exponentially slow dynamics.

- FitzHugh-Nagumo: No coarsening, no mass conservation [Goldstein, Muraki, Petrich, 96]

Final comment

Localized structures far from the Turing regime are commonplace in reaction-diffusion systems such as the Brusselator, and provide an alternative pattern-formation mechanism to Turing instability.

Turing analysis cannot explain the diverse phenomena that can occur in this regime, such as coarsening and the “breather”-type instabilities. However singular perturbation tools can be successfully applied to asnwer many of these questions.