Coarsening and self-replication of mesa patterns in reaction-diffusion systems

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Joint work with

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Highlights of past work

- 1952, Turing; 1968-2006, Prigogine, Lefever, Brusselator, weakly nonlinear Turing analysis
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- 1994, Lee, McCormick, Pearson and Swinney: experimental verification
- 1994-2006: Self-replication observed experimentally and numerically in other chemical/biological systems:
  - Ferrocyanide-iodide-sulfite reaction (Lee, Swinney)
  - Belousov-Zhabotinsky reaction (Muñuzuri, Pérez-Villar Markus)
  - Bonhoffer-van der Pol system (Hayase, Ohta)
  - Gierer-Meinhardt model (Meinhardt)
Some examples of patterns in 2-D

Dynamic patterns: coarsening

In 1-D:
Dynamic patterns: coarsening

In 2-D:
Dynamic patterns: self-replication

In 1-D:
Dynamic patterns: self-replication

In 2-D:
Dynamic patterns: Breather
Part 1: Coarsening and oscillatory behaviour
The Brusselator model

Rate equations:

\[ A \rightarrow X, \quad B + X \rightarrow Y + C, \quad 2X + Y \rightarrow 3X, \quad X \rightarrow E. \]
The Brusselator model

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A^{\text{slow}} \rightarrow X, \quad B + X \rightarrow Y + C, \quad 2X + Y \rightarrow 3X, \quad X^{\text{slow}} \rightarrow E.
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After rescaling, we get a PDE system:

\[ u_t = \varepsilon^2 u_{xx} - u + \alpha + u^2 v \]

\[ \tau v_t = \varepsilon^2 v_{xx} + (1 - \beta) u - u^2 v. \]
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In terms of total mass \( w = u + v \), steady state becomes

\[ 0 = \varepsilon^2 u'' - u + \alpha + u^2 (w - u) \]
\[ 0 = \varepsilon^2 w'' + \alpha - \beta u. \]
Slow-fast structure

Introduce

\[ \beta_0 \equiv \beta / \alpha, \quad D \equiv \varepsilon^2 / \alpha \]

and assuming \( \alpha \) small, the steady state problem becomes

\begin{align*}
0 &= \varepsilon^2 u'' - u + u^2(w - u) \\
0 &= Dw'' + 1 - \beta_0 u.
\end{align*}

\[ w'(0) = w'(L) = u'(0) = u'(L) = 0 \]

and we assume

\[ \varepsilon \ll 1, \quad \varepsilon^2 \ll D, \quad \beta_0 = O(1). \]

Then \( w \) is slow and \( u \) is fast.
Construction of a half-mesa, $D \gg 1$

\[
0 = \varepsilon^2 u'' - u + u^2(w - u) \\
0 = Dw'' + 1 - \beta_0 u.
\]

\[
w'(0) = 0 = w'(L), \quad u'(0) = 0 = u'(L)
\]

Expand in $\frac{1}{D}$, then to leading order $w(x) \sim w_0$; and

\[
\varepsilon^2 u'' \sim f(u, w_0) \equiv u - u^2(w_0 - u)
\]

Moreover, \( \int_0^L u = \frac{L}{\beta_0} = O(1) \). So \( f(u, w_0) \) must satisfy the **maxwell line condition**, \( \int_0^{u^*} f(u) du = 0 \) where \( f(u^*) = 0 \).

\[
\implies u^* = \sqrt{2}; \quad w_0 = \frac{3}{\sqrt{2}}.
\]
Construction of a half-mesa, $D \gg 1$

... $w(x) \sim \frac{3}{\sqrt{2}}$; $u(x) \sim \begin{cases} 
  u^* = \sqrt{2}, & 0 < x < x_0 \\
  0, & x > x_0 
\end{cases}$

\[
  u \sim \frac{1}{\sqrt{2}} \left( 1 - \tanh \left( \frac{x - x_0}{2\epsilon} \right) \right), \quad x \in (0, L)
\]

To determine $x_0$: \( \int_0^L u \sim u^* x_0 = \frac{L}{\beta_0} \implies x_0 \sim \frac{L}{\sqrt{2} \beta_0} \).
Construction of multiple mesas

- Replace $L$ by $2L$ and use reflection:

- Replace $L$ by $KL$ and use translation, reflection,
Stability of $K$ mesas, $K^{-2} \ll D \ll O \left( \varepsilon^2 \exp \left( \frac{1}{\varepsilon K} \right) \right)$

**Theorem 1.** Consider a $K$ mesa equilibrium state on $[0, 1]$ with $K^{-2} \ll D \ll O \left( \varepsilon^2 \exp \left( \frac{1}{\varepsilon K} \right) \right)$. There are $2K$ small eigenvalues of order $O \left( \frac{\varepsilon^2}{D} \right)$; all other eigenvalues are negative and have order $\leq O \left( \varepsilon^2 \right)$. The smallest $2K$ eigenvalues are given by

$$\lambda_{j\pm} \sim -\frac{\varepsilon^2}{D \beta_0 (1 - \tau)} \left( 1 \mp \sqrt{1 - 2K^2 dl \left[ 1 - \cos \left( \frac{\pi j}{K} \right) \right]} \right), \quad j = 1 \ldots K - 1;$$

$$\lambda_- \sim -\frac{\varepsilon^2}{D \beta_0 (1 - \tau)} Kl, \quad \lambda_+ \sim -\frac{\varepsilon^2}{D \beta_0 (1 - \tau)} l.$$

Here, $l = \frac{\sqrt{2}}{\beta_0 K}$; $d = \frac{1}{K} - l$. All eigenvalues are negative when $\tau > 1$, and positive when $\tau < 1$. The transition from stability to instability occurs via a Hopf bifurcation as $\tau$ is decreased past $\tau_h$ where to leading order, $\tau_h \sim 1$. 
Theorem 2. Let

\[ D_K \sim \frac{(\sqrt{2}\beta_0 - 1)^2}{12\sqrt{2}\beta_0} \varepsilon^2 \exp \left( \frac{1}{\varepsilon K \sqrt{2\beta_0^3}} \right). \]

Then \( K \)-mesa solution is unstable provided that \( D > D_K \).
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More precise, implicit formula is available.
Instability for exponentially large $D$

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- More precise, implicit formula is available.
- This threshold is responsible for the coarsening process.
Example of Theorem 2

\[ \beta_0 = 2.8, \varepsilon = 0.01, D = 10; \]
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From Theorem 2,

\[ D_1 = 5 \times 10^6, \]
\[ D_2 = 15.7, \]
\[ D_3 = 0.23. \]

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No more coarsening will be observed.

\[ \beta_0 = 2.8, \varepsilon = 0.01, D = 10; \]
Scaling laws

- The characteristic width of the interface is $O(\varepsilon)$.
- The threshold at which coarsening occurs is of order
  \[
  \frac{D}{\varepsilon^2} \sim O\left(\exp\left(\frac{c}{K\varepsilon}\right)\right).
  \]
- For this $D$, the exponentially small tails of $u$ are of the same order as $w$. This causes instability.
Consider a single symmetric mesa solution on domain \([0, L]\). Second order computation yields,

\[
w(L) \sim \frac{3}{\sqrt{2}} + (1 - \sqrt{2}\beta_0)\beta_0^2 L^2 + 3\sqrt{2} \left( \exp \left( \frac{-2l}{\epsilon} \right) + \exp \left( \frac{-2d}{\epsilon} \right) \right)
\]
By gluing, two-mesa asymmetric solution is constructed on interval of length $1.4 = 0.6 + 0.8$ (red line).

For interval length $1.1$, only symmetric solution is possible (green line, $1.1 = 0.55 + 0.55$).

Asymmetric branch bifurcates from symmetric at $L \sim 1.4 = 2 \times 0.7$. 
Let $L^*$ be minimum of the curve $L \rightarrow w(L)$ (here $L^* = 0.7$).

At that point an asymmetric solution bifurcates from the symmetric branch.

This point coincides with the instability threshold for $K$ mesas after setting $L = KL^*$. 
Comparison with Turing instability

From Theorem 2, coarsening occurs whenever

\[ K > K^* = O \left( \frac{1}{\varepsilon \ln \left( \frac{D}{\varepsilon^2} \right)} \right), \quad D \gg 1. \]
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- $k^* \gg K^*$ by a logarithmically large amount. Therefore initial Turing instability is always followed by the coarsening process.
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- \( k^* \gg K^* \) by a logarithmically large amount. Therefore initial Turing instability is always followed by the coarsening process.

- Numerical simulations suggest that this is also true in 2-D. click here
**Breather-type instability**

*Theorem 3.* Suppose that $D \ll \varepsilon^2 \exp \left( \frac{c}{\varepsilon} \right)$. Then all small eigenvalues undergo a Hopf bifurcation as $\tau$ is increased past 1. If in addition

$$\frac{1}{\varepsilon} \ll D$$

then the first mode to undergo a Hopf bifurcation is the mode $\lambda_+$. This occurs at $\tau$ is increased past

$$\tau_{h+} = 1 - \frac{\beta_0}{4D} \left( ld - \frac{K}{3} (d^3 + l^3) \right).$$

The corresponding eigenvalue has value

$$\lambda_+ \sim i \sqrt{\frac{8K \beta_0 \varepsilon^3}{D}}.$$
Theorem 3 gives $\lambda_+ \sim 0.0168$ so that one period is $P = \frac{2\pi}{\lambda_+} \sim 373.5$. This agrees with an estimate $P \sim 400$ from the figure.
Part 2: Self-replication, \( D = O(1) \).
Steady state, Outer region

\[ 0 = \varepsilon^2 u_{xx} - u + u^2 (w - u); \quad 0 = Dw_{xx} + 1 - \beta_0 u \]

Neglect \( \varepsilon^2 u_{xx} \). Then

\[ w \sim \frac{1}{u} + u \equiv g(u); \]

\[ Dw_{xx} = \beta_0 g^{-1}(w) - 1 \]

So \( u \) is slave to \( w \) in the outer region.
Steady state, Inner region

\[ 0 = \varepsilon^2 u_{xx} - u + u^2(w - u); \quad 0 = Dw_{xx} + 1 - \beta_0 u \]

Rescale

\[ y = \frac{x - x_0}{\varepsilon}; \]

then \( w_{yy} \sim 0 \) so that to leading order,

\[ w(y) \sim w_0; \quad u_{yy} = f(u) \equiv u - u^2(w_0 - u). \]

Impose the Maxwell line condition (the areas between roots of \( f \) are equal); obtain

\[ w(x_0) \sim \frac{\sqrt{3}}{2}; \quad u(x_0) \sim \sqrt{2}. \]
Steady state, matching

\[ 0 = \varepsilon^2 u_{xx} - u + u^2(w - u); \quad 0 = Dw_{xx} + 1 - \beta_0 u \]

Solve

\[ Dw_{xx} = \beta_0 g^{-1}(w) - 1, \quad x \in (0, x_0) \]

where \( g(u) = \frac{1}{u} + u \) subject to

\[ w'(0) = 0, \quad w(x_0) = g(\sqrt{2}) = \frac{3}{\sqrt{2}}, \quad \int_0^{x_0} u = \frac{L}{\beta_0}. \]
Dissapearence of steady state

- There exists $D_c = O(1)$ such that no outer solution exists for $D < D_c$.
- When $D = D_c$, $w(0)$ corresponds to a minimum of $w = g(u) = \frac{1}{u} + u$,

  $$w(0) \sim 2; \quad u(0) \sim 1 \quad \text{when} \quad D = D_c.$$

- A boundary layer forms near $x = 0$ when $D \sim D_c$. 
The core problem

The solution within the boundary is described by a core problem,

\[ U''(y) = U^2 - A - y^2; \quad U'(0) = 0, \quad U' \to 1 \quad \text{as} \quad y \to \infty. \] (1)

The proof of self-replication is reduced to the study of this core problem.

We rigorously show the existence of fold-point bifurcation for (1). This provides a connection between single and double mesa pattern, leading to pulse splitting.
Universality of the Core Problem

- Mesa-type patterns are common in many systems.
- Some other models that exhibit mesa self-replication are:
  - Lengyel & Epstein model:
    \[ u_t = \varepsilon^2 u_{xx} - u + a - \frac{4uv}{1 + u^2}; \quad \tau v_t = Dv_{xx} + b \left( u - \frac{uv}{1 + u^2} \right) \]
  - Gierer-Meinhardt model with saturation:
    \[ a_t = \varepsilon^2 a_{xx} - a + \frac{a^2}{h(1 + \kappa a^2)}; \quad \tau h_t = Dh_{xx} - h + a^2 \]
- Both of these systems have self-replication thresholds
- The same core problem appears at that threshold.
Universality of the Core Problem

epstein model:
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]
Open question 1

Study the limit where a mesa becomes a spike ($\beta_0 \to 0$)

- Self-replication may still occur but the core problem is more complicated.
- Coarsening regime disappears?
- Oscillatory behaviour changes. Thresholds?

![Graph showing the behavior of a mesa as $\beta_0$ approaches 0.](image)
Open question 2

Describe the slow dynamics of the mesas. There are two types:

- slow mass exchange \((t \sim 0 - 2000)\)
- slow motion \((t > 2200)\)
Open question 3

Study the Brusselator in 2D or 3D.
- Coarsening in 2D
- Stability of a disk, ring or stripe
- Can one obtain labyrinthian patterns?
Some References


These can be downloaded from my website, http://www.mathstat.dal.ca/~tkolokol