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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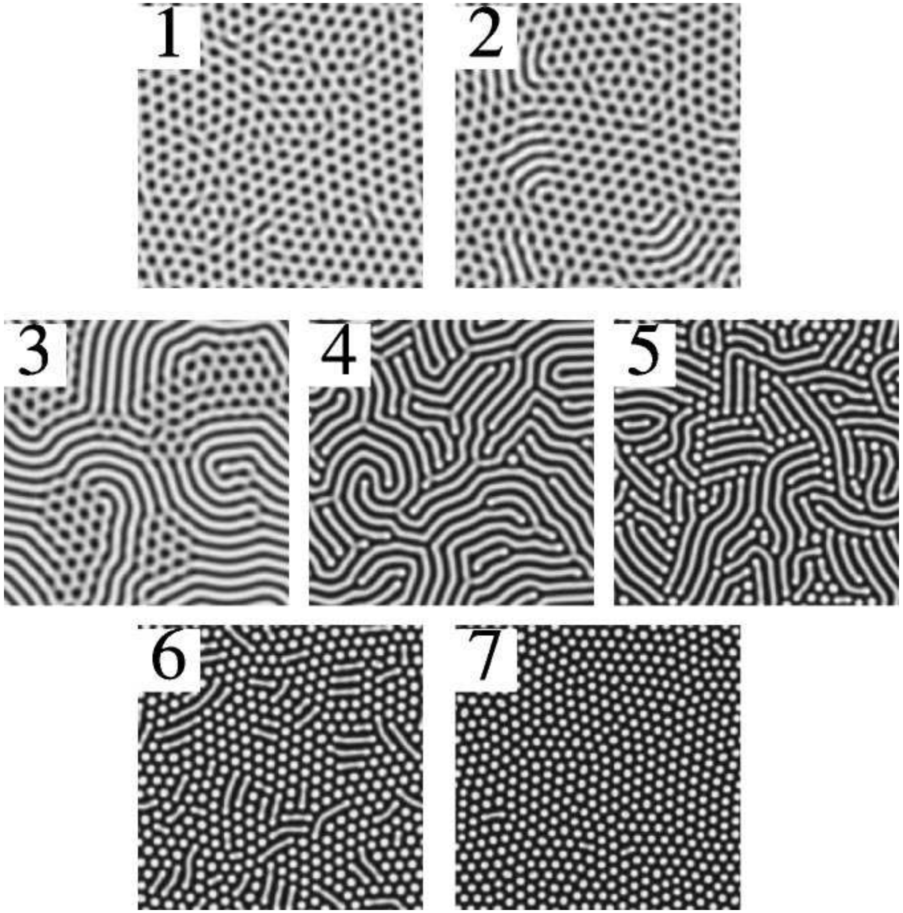
- 1994, Lee, McCormick, Pearson and Swinney: experimental verification
- 1994-2006: Self-replication observed experimentally and numerically in other chemical/biological systems:
  - Ferrocyanide-iodide-sulfite reaction (Lee, Swinney)
  - Belousov-Zhabotinsky reaction (Muñuzuri, Pérez-Villar Markus)
  - Bonhoffer-van der Pol system (Hayase, Ohta)
  - Gierer-Meinhardt model (Meinhardt)

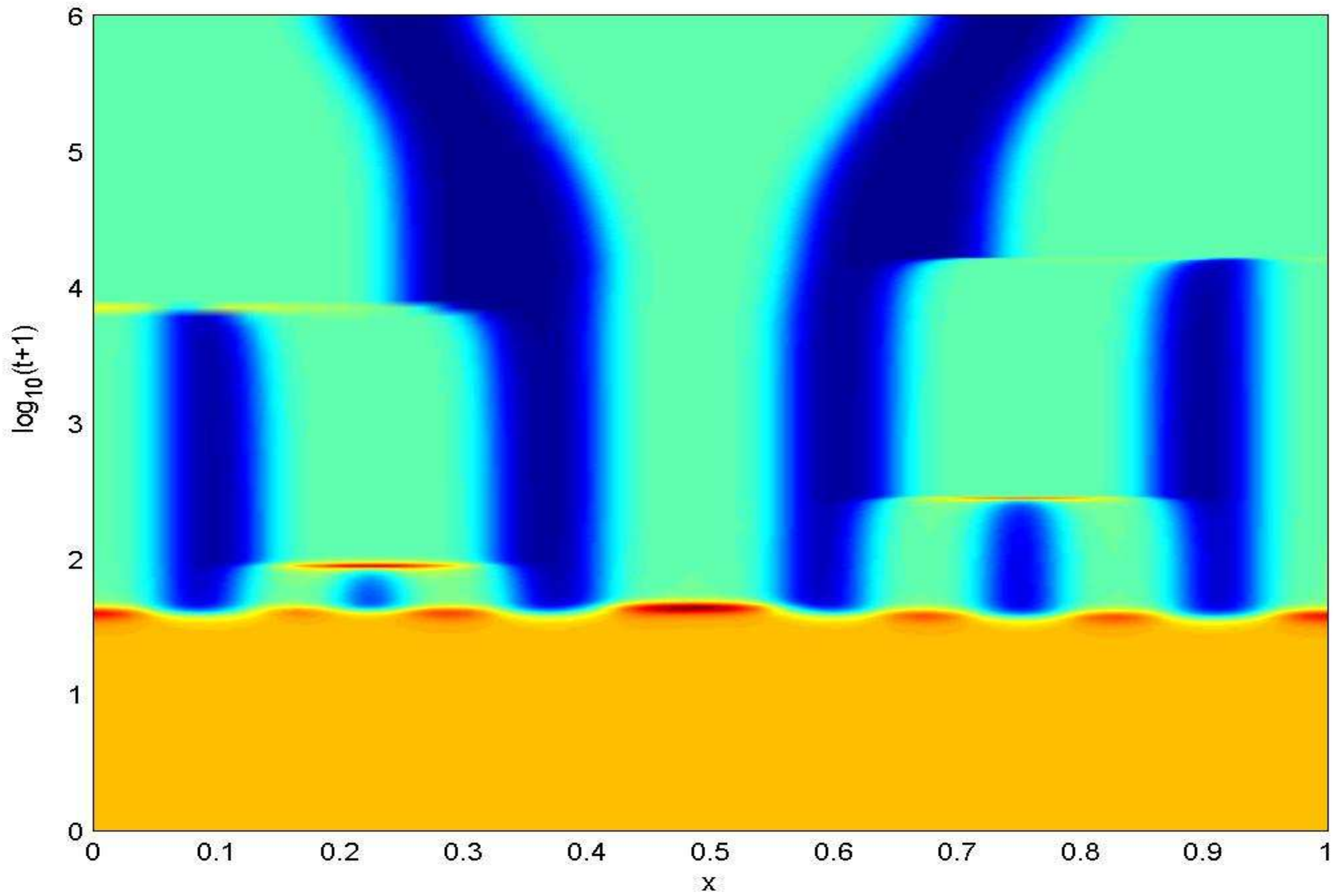
Some examples of patterns in 2-D



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

Dynamic patterns: coarsening

In 1-D:

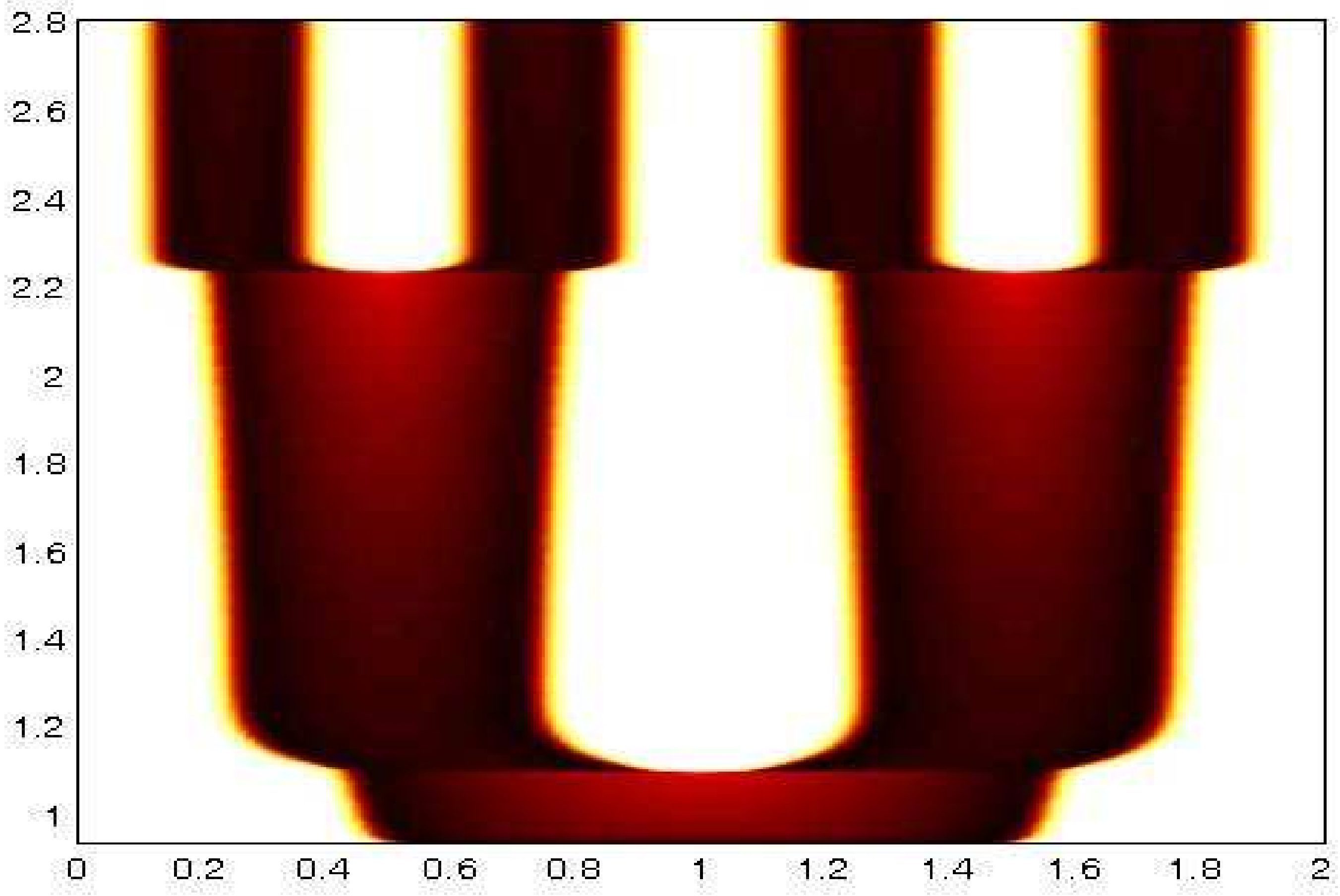


Dynamic patterns: coarsening

In 2-D:

Dynamic patterns: self-replication

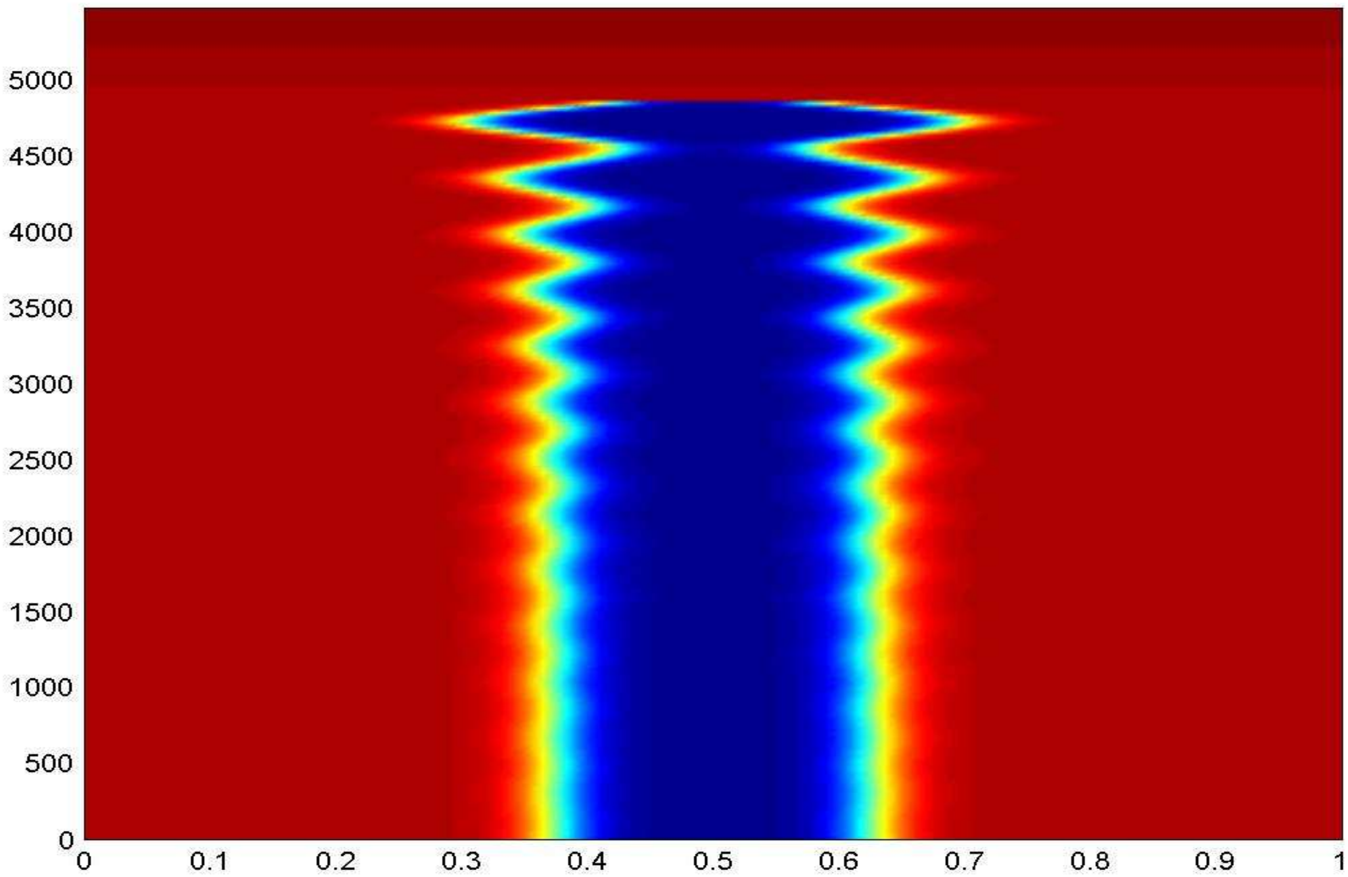
In 1-D:



Dynamic patterns: self-replication

In 2-D:

Dynamic patterns: Breather



Part 1: Coarsening and oscillatory behaviour

The Brusselator model

Rate equations:

$$A \;\to\; X, \quad B + X \to Y + C, \quad 2X + Y \to 3X, \quad X \;\to\; E.$$

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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

$$\beta_0 \equiv \frac{\beta}{\alpha}, \quad D \equiv \frac{\varepsilon^2}{\alpha}$$

and assuming α small, the steady state problem becomes

$$\boxed{\begin{aligned} 0 &= \varepsilon^2 u'' - u + u^2(w-u) \\ 0 &= Dw'' + 1 - \beta_0 u. \\ w'(0) &= w'(L) = u'(0) = u'(L) = 0 \end{aligned}}$$

and we assume

$$\varepsilon \ll 1, \;\; \varepsilon^2 \ll D, \;\; \beta_0 = O(1).$$

Then w is slow and u is fast.

Construction of a half-mesa, $D \gg 1$

$$0 = \varepsilon^2 u'' - u + u^2(w - u)$$

$$0 = Dw'' + 1 - \beta_0 u.$$

$$w'(0) = 0 = w'(L), \;\; u'(0) = 0 = u'(L)$$

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

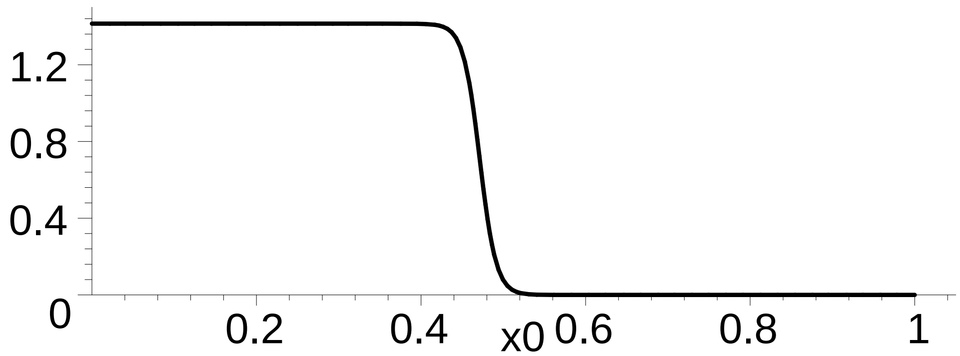
$$\varepsilon^2 u'' \sim f(u, w_0) \equiv u - u^2(w_0 - u)$$

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

$$\implies u^\star = \sqrt{2}; \;\; w_0 = \frac{3}{\sqrt{2}}.$$

Construction of a half-mesa, $D \gg 1$

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

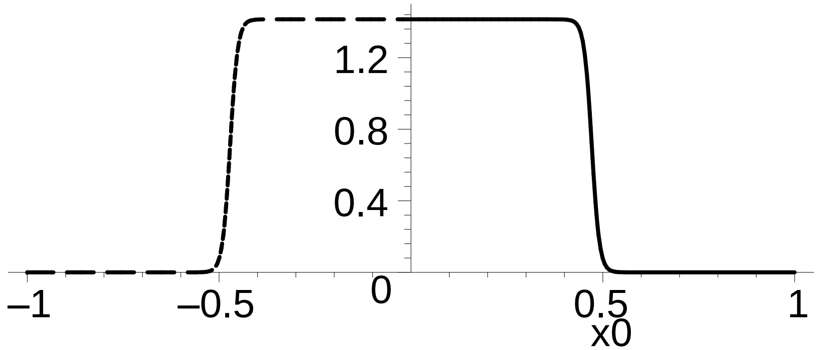


$$u \sim \frac{1}{\sqrt{2}}\left(1 - \tanh\left(\frac{x - x_0}{2\varepsilon}\right)\right), \quad x \in (0, L)$$

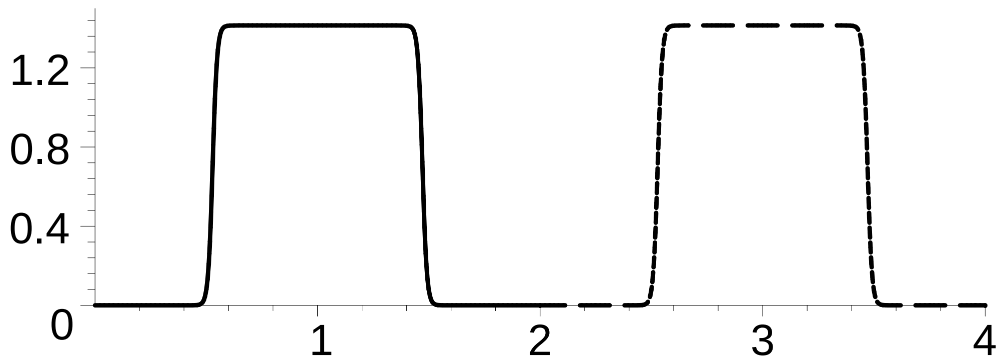
To determine x_0: $\int_0^L u \sim u^\star x_0 = \frac{L}{\beta_0} \implies \boxed{x_0 \sim \frac{L}{\sqrt{2}\beta_0}.}$

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

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

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

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 τ is decreased past τ_h where to leading order, $\tau_h \sim 1$.

Instability for exponentially large D

Theorem 2. Let

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

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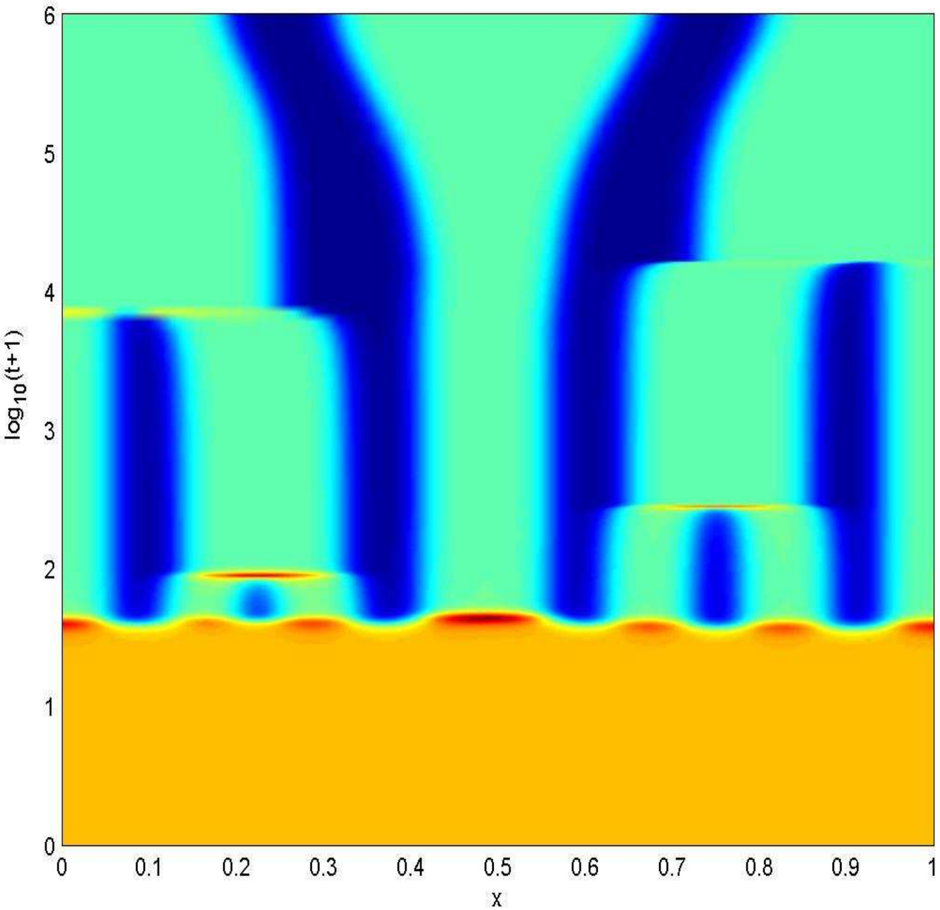
- More precise, implicit formula is available.
- This threshold is responsible for the coarsening process.

Example of Theorem 2



$\beta_0 = 2.8, \varepsilon = 0.01, D = 10;$

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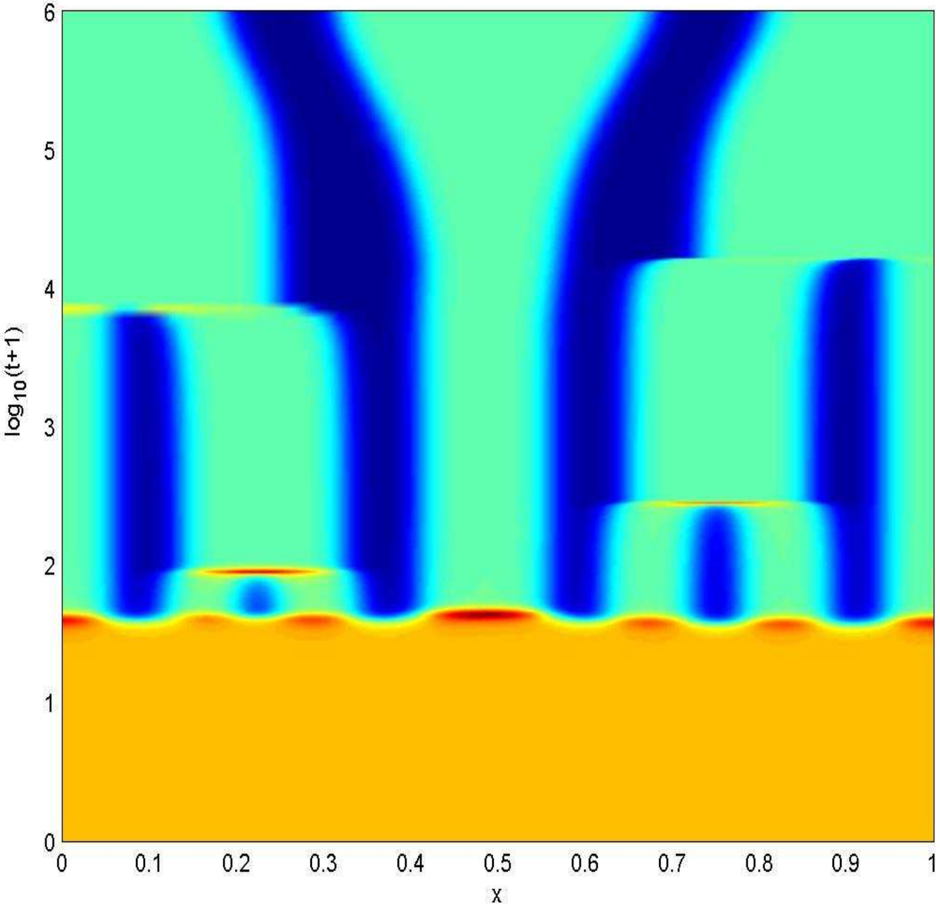

- From Theorem 2,

$$D_1 = 5 \times 10^6,$$

$$D_2 = 15.7,$$

$$D_3 = 0.23.$$

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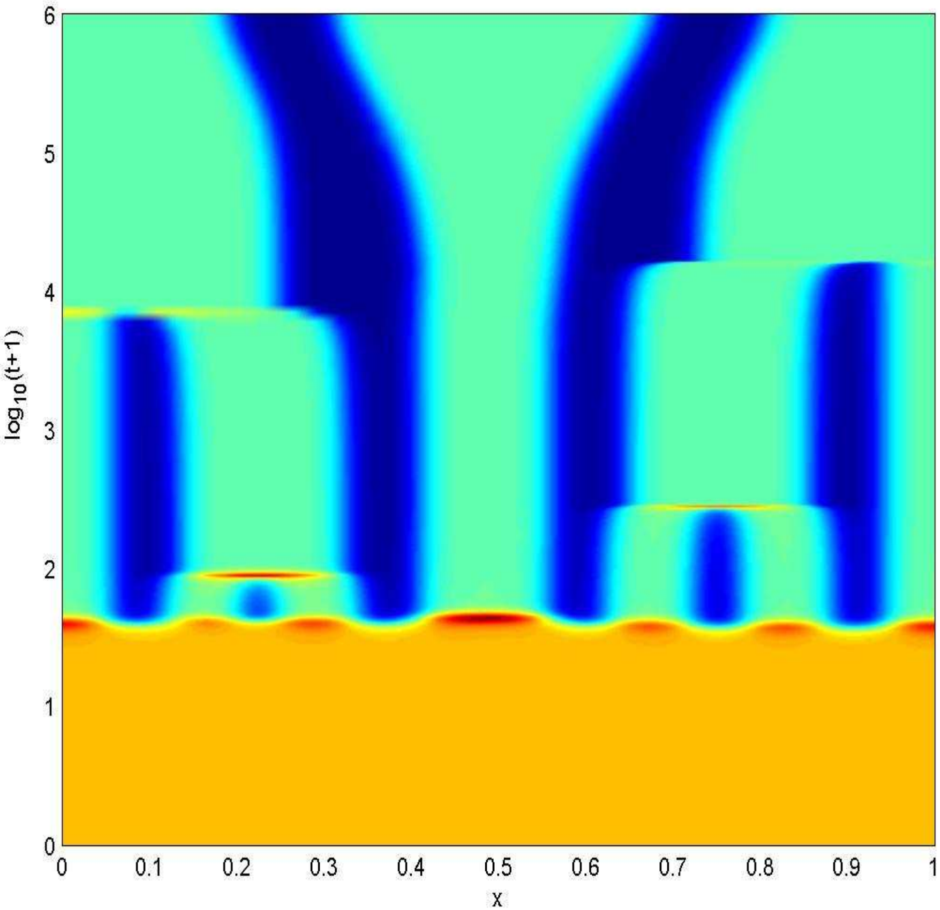

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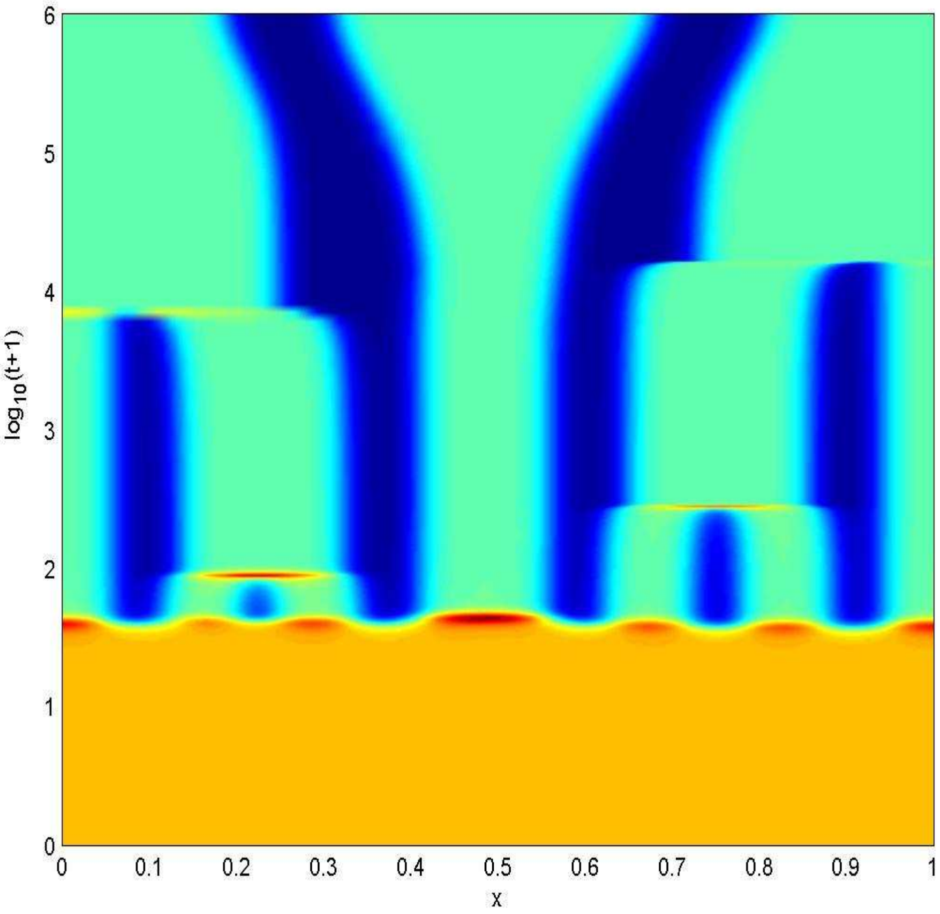

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- $D_3 < D < D_2 \implies K = 2$ is stable but $K = 3$ unstable.
- No more coarsening will be observed.

Scaling laws

- The characterisitic width of the interface is $O(\varepsilon)$.
- The threshold at which coarsening occurs is of order

$$\frac{D}{\varepsilon^2} \sim O\left(\exp\left(\frac{c}{K\varepsilon}\right)\right).$$

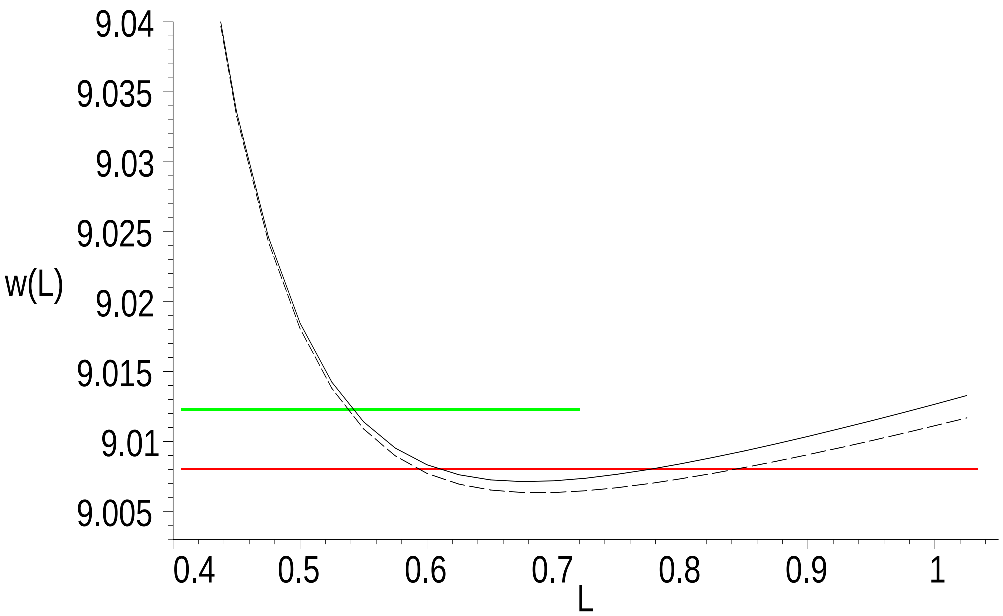
- For this D, the exponentially small tails of u are of the same order as w. This causes instability.

Coarsening and Asymmetric patterns

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

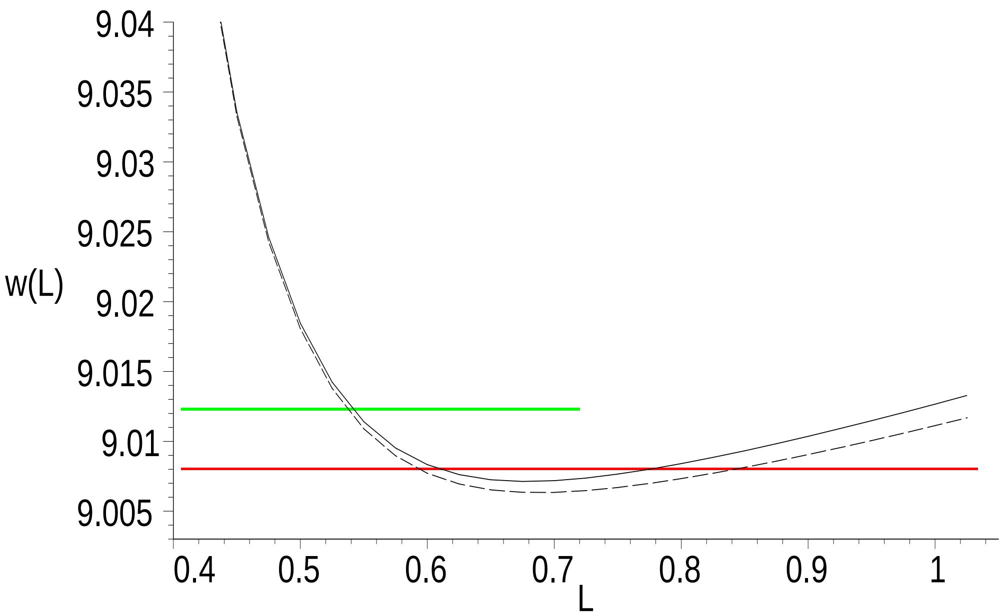
$$w(L) \sim \frac{3}{\sqrt{2}} + (1 - \sqrt{2}\beta_0)\beta_0^2 L^2 + 3\sqrt{2}\left(\exp\left(\frac{-2l}{\varepsilon}\right) + \exp\left(\frac{-2d}{\varepsilon}\right)\right)$$

Asymmetric patterns: example



- By glueing, 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 $L \sim 1.4 = 2 \times 0.7$.

"Proof" of Theorem 2



- Let $L^\star$ be minimum of the curve $L \to w(L)$ (here $L^\star = 0.7$).
- At that point an asymmetric solution bifurcates from the symmetric branch.
- This point coincides with the instability threshold for K mesas after setting $L = KL^\star$.

Comparison with Turing instability

- From Theorem 2, coarsening occurs whenever

$$K > K^{\star} = O\left(\frac{1}{\varepsilon}\frac{1}{\ln\left(\frac{D}{\varepsilon^2}\right)}\right), \quad D \gg 1.$$

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- $k^{\star} \gg K^{\star}$ 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 bifrcation as τ is increased past 1. If in addition

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

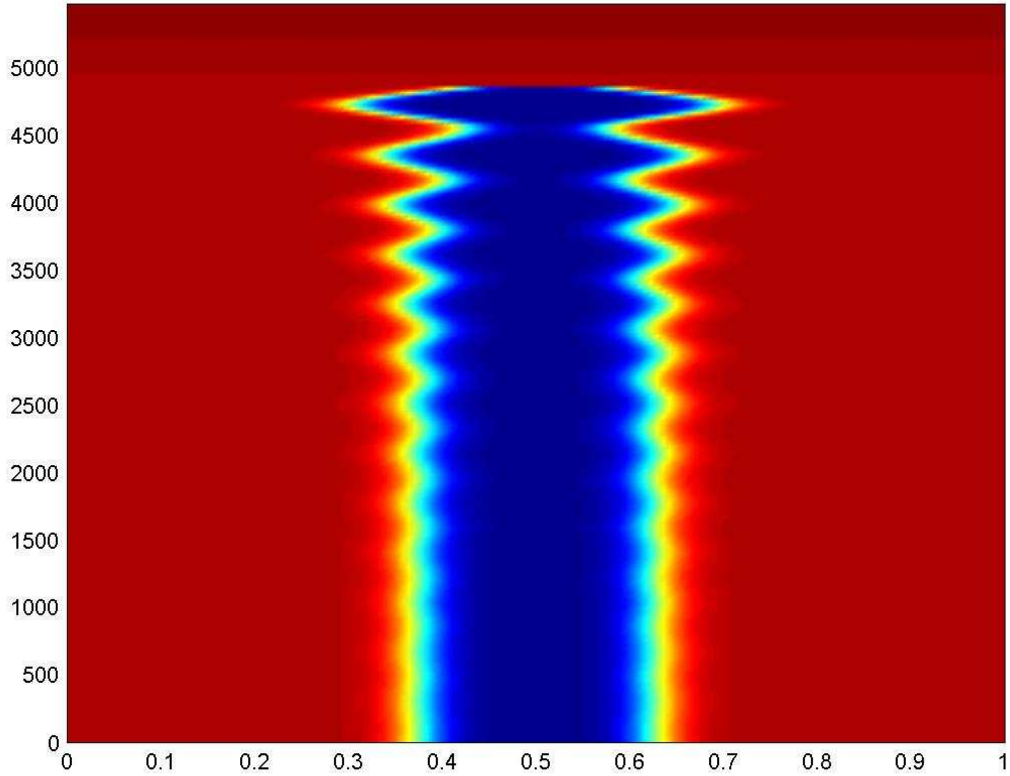
then the first mode to undergo a Hopf bifurcation is the mode λ_+. This occurs at τ is increased past

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

The corresponding eigenvalue has value

$$\lambda_+ \sim i\sqrt{\frac{8K\beta_0\varepsilon^3}{D}}.$$

Breather-type instability: example



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

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

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

$$0 = \varepsilon^2 u_{xx} - u + u^2(w - u); \qquad 0 = D w_{xx} + 1 - \beta_0 u$$

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

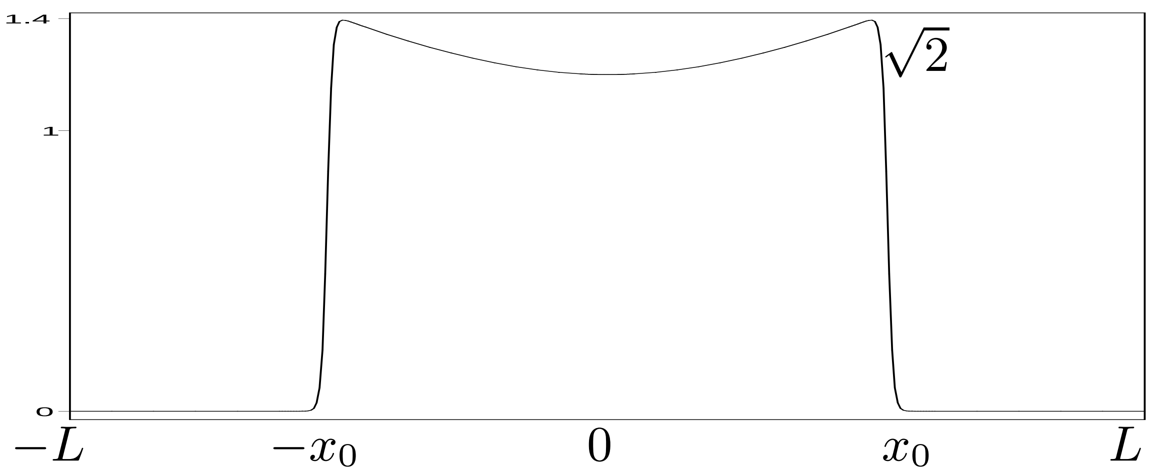
$$0 = \varepsilon^2 u_{xx} - u + u^2(w-u); \qquad 0 = Dw_{xx} + 1 - \beta_0 u$$

Solve

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

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

$$w'(0) = 0, \quad w(x_0) = g(\sqrt{2}) = \frac{3}{\sqrt{2}}, \qquad \int_0^{x_0} u = \frac{L}{\beta_0}.$$

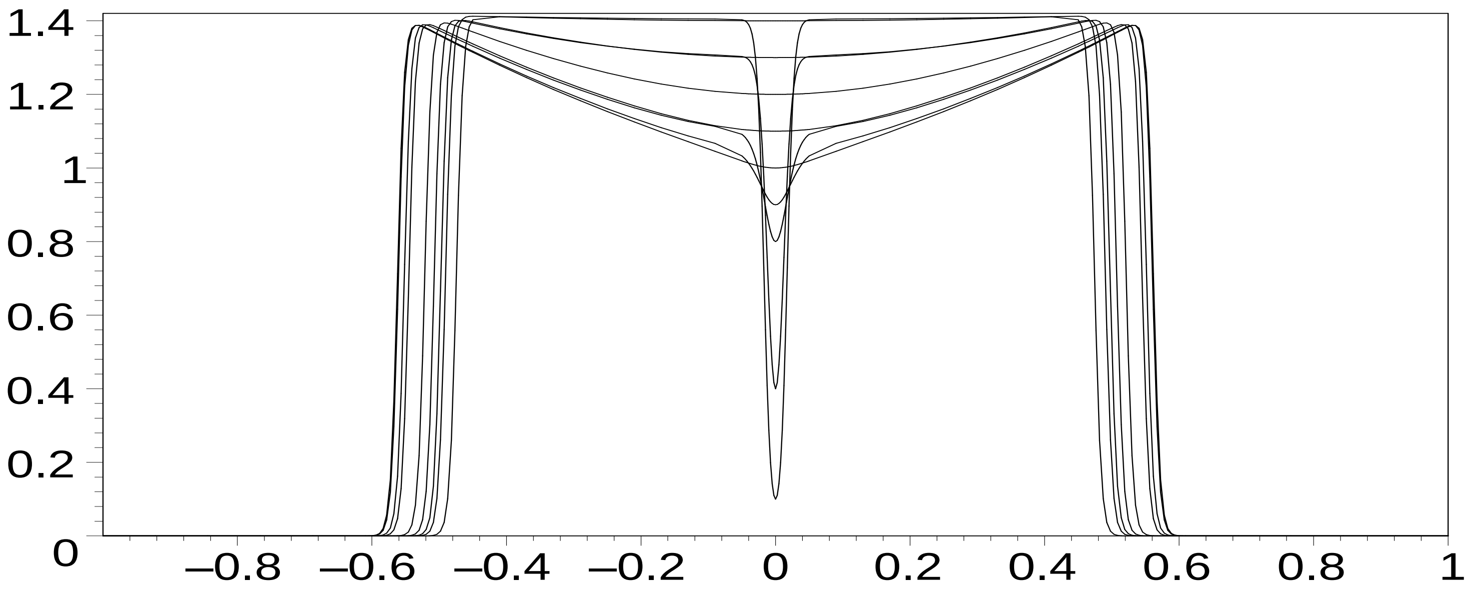


Dissapearence of steady state

- 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*,

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

- The proof of self-replication is reduced to the study of this core problem
- We rigorously show the existence of fold-point bifurcaiton 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:

$$u_t = \varepsilon^2 u_{xx} - u + a - \frac{4uv}{1+u^2}; \quad \tau v_t = D v_{xx} + b\left(u - \frac{uv}{1+u^2}\right)$$

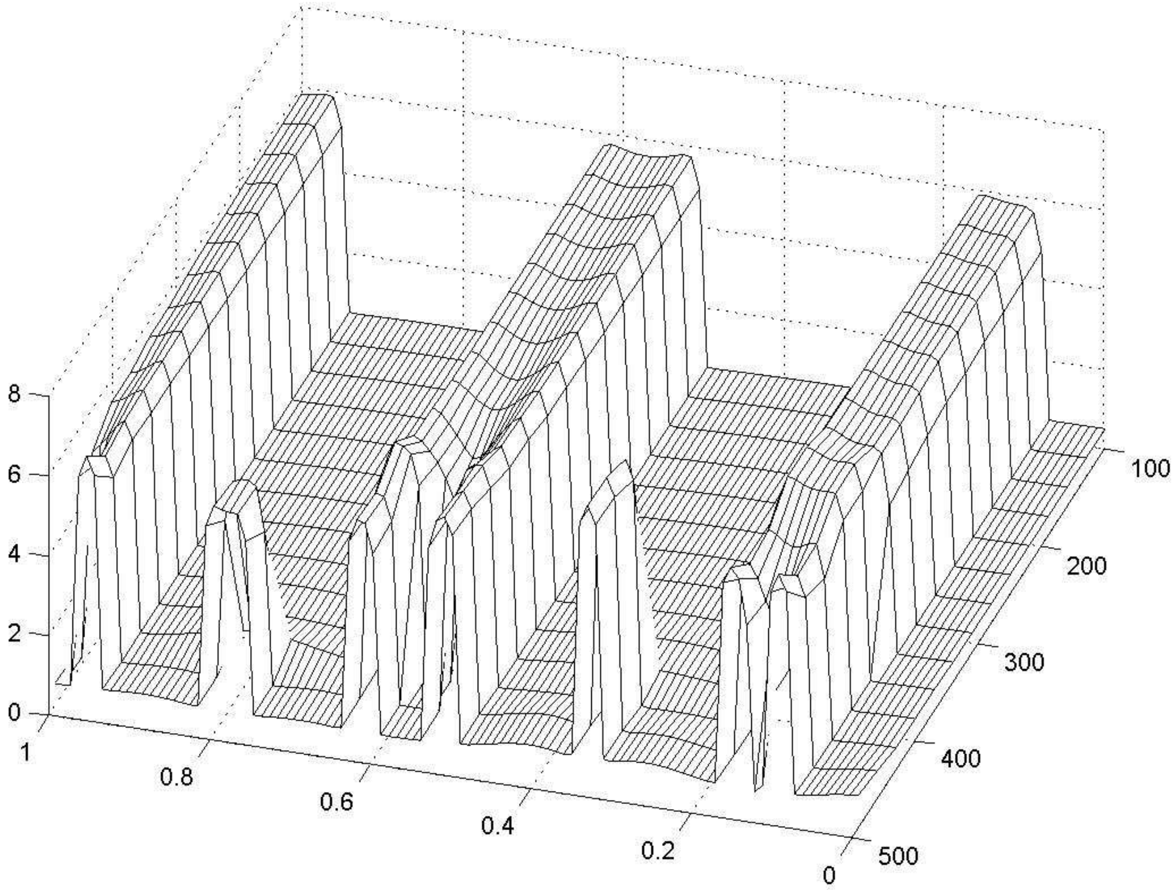
  - Gierer-Meinhardt model with saturation:

$$a_t = \varepsilon^2 a_{xx} - a + \frac{a^2}{h(1+\kappa a^2)}; \quad \tau h_t = D h_{xx} - h + a^2$$

- Both of these systems have self-replication thresholds
- The same core problem appears at that threshold.

Universality of the Core Problem

Epstein model:



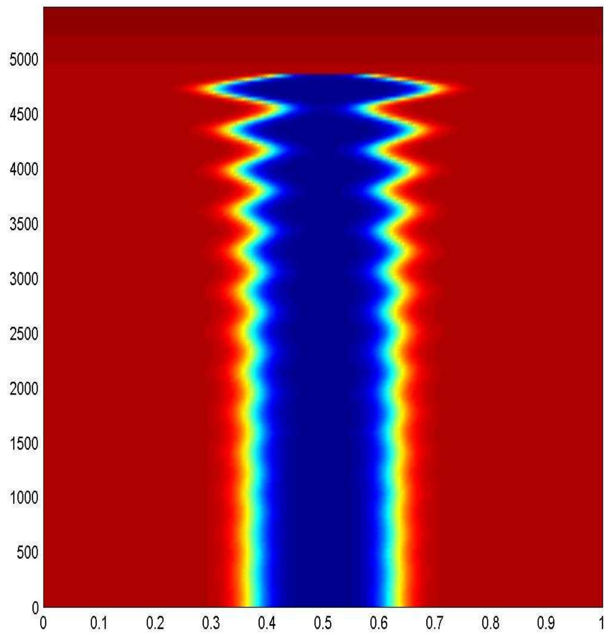
Comparison to other bistable systems

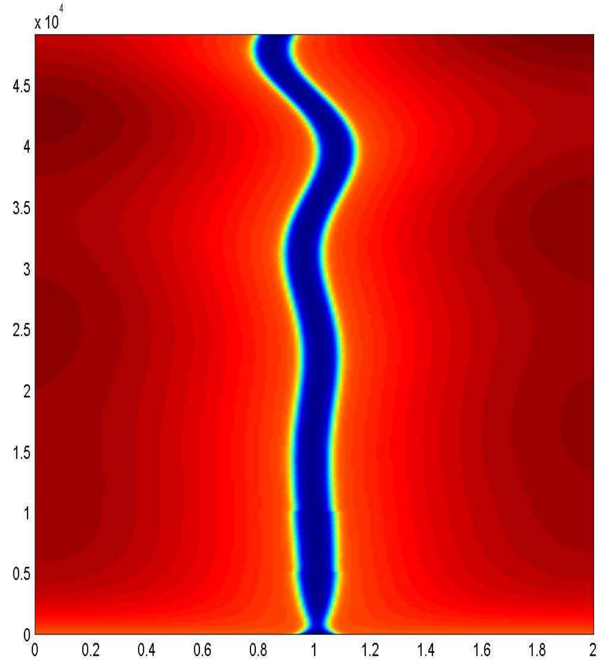
- Brusselator: Has an asymptotic “mass conservation” law. Coarsening process terminates when $K = K^* \gg 1$. Algebraically slow dynamics?
- Cahn-Hilliard: Has a variational structure, exact mass conservation. Coarsening proceeds until only one interface is left. Exponentially slow dynamics.
- FitzHugh-Nagumo: 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 dissapears?
- Oscillatory behaviour changes. Thresholds?

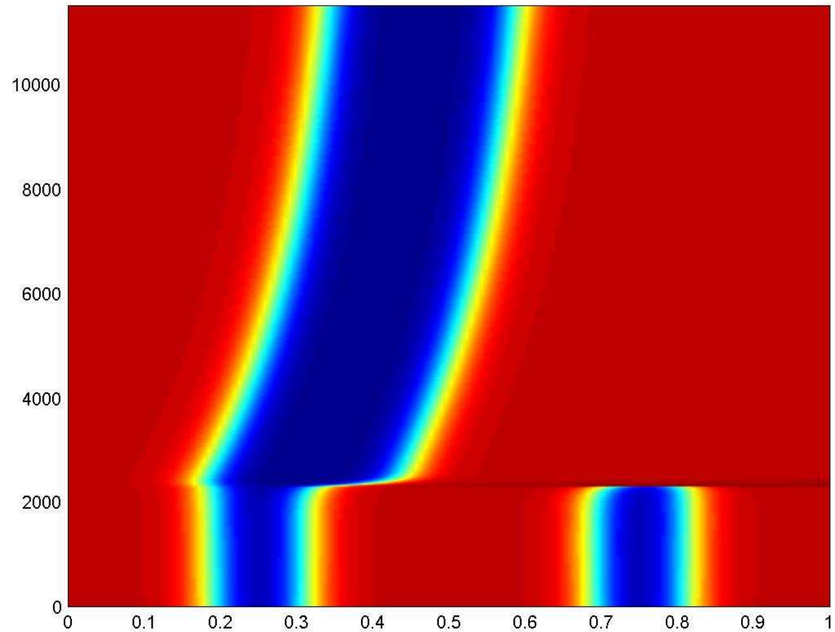




Open question 2

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 labrynthian patterns?

Some References

- T. Kolokolnikov, T. Erneux and J. Wei, *Mesa-type patterns in the one-dimensional Brusselator and their stability*, Physica D 214(2006) 63-77.
- T. Kolokolnikov, T. Erneux, and J. Wei, *Self-replication of mesas in reaction-diffusion models*, preprint
- T. Kolokolnikov, M.J. Ward and J. Wei, *The Stability of a Stripe for the Gierer-Meinhardt Model and the Effect of Saturation*, to appear, SIAM J. Appl. Dyn. Systems.

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