Self-replication of mesa patterns in reaction-diffusion systems

Theodore Kolokolnikov
Dalhousie University

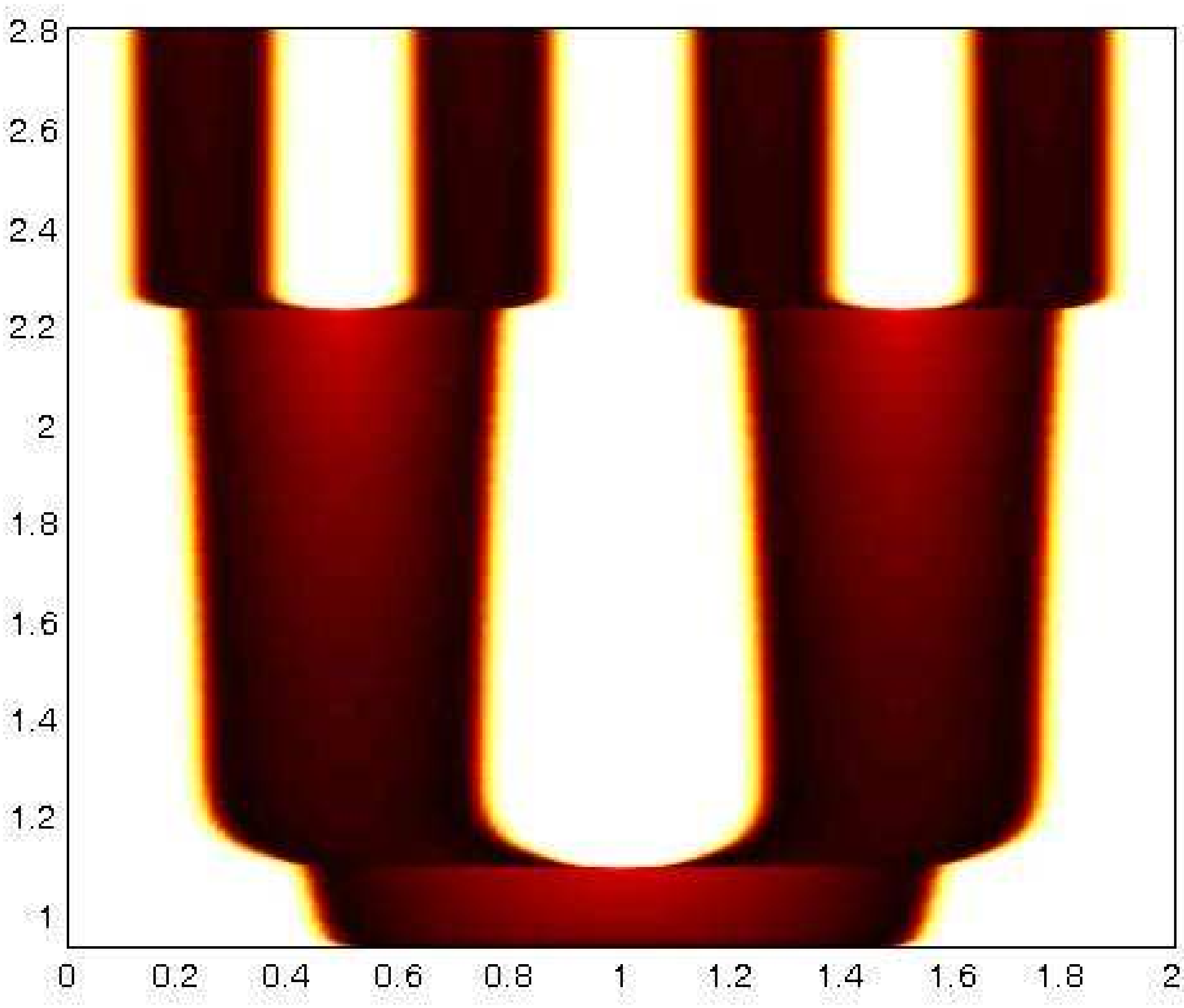
Joint work with

Juncheng Wei
Michael Ward

Highlights of past work

- 1994, Pearson: self-replication in Gray-Scott model. Also observed a zoo of different patterns: spots, stripes, hexagonal patterns, oscillatory instabilities, spatio-temporal chaos...
- 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 (Vanag, Epstein, Muñuzuri, Pérez-Villar Markus)
  - Bonhoffer-van der Pol system (Hayase, Ohta)
  - Gierer-Meinhardt model (Meinhardt)
  - Gray-Scott model (Doelman, Kaper, Muratov, Osipov, Kolokolnikov, Ward, Wei)

Part I: Self-replication in 1D



The Brusselator model

Rate equations:

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

After rescaling, we get a PDE system:

$$u_t = \varepsilon^2 u_{xx} - u + \alpha + u^2 v$$
$$\tau v_t = \varepsilon^2 v_{xx} + (1 - \beta)\, u - u^2 v.$$

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

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

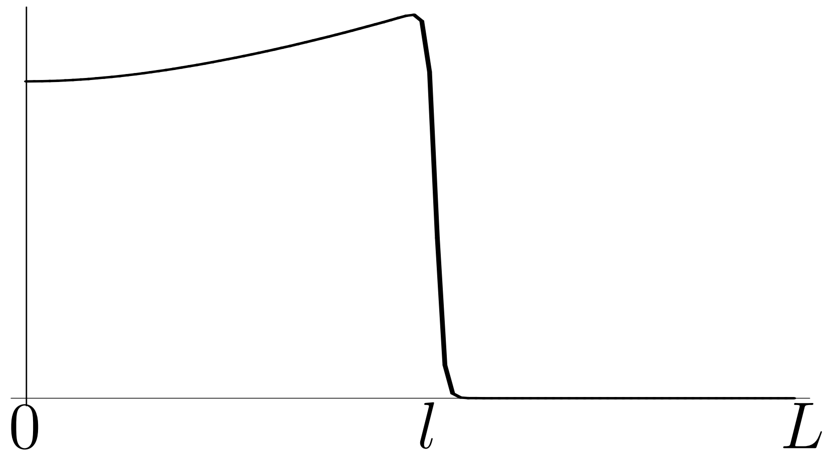
and we assume

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

Then w is slow and u is fast.

Steady state

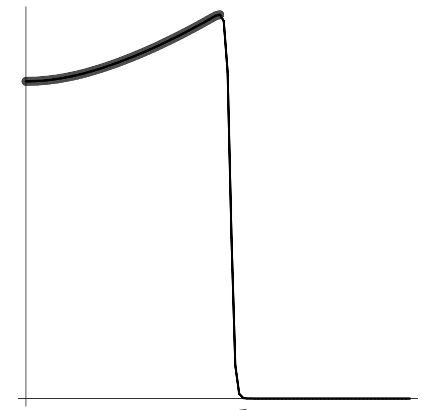
$$0 = \varepsilon^2 u_{xx} - u + u^2(w - u); \qquad 0 = D w_{xx} + 1 - \beta_0 u$$



- Analyse the inner and outer region separately
- Use asymptotic matching.

Steady state: Outer region

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



Neglect $\varepsilon^2 u_{xx}$. Then

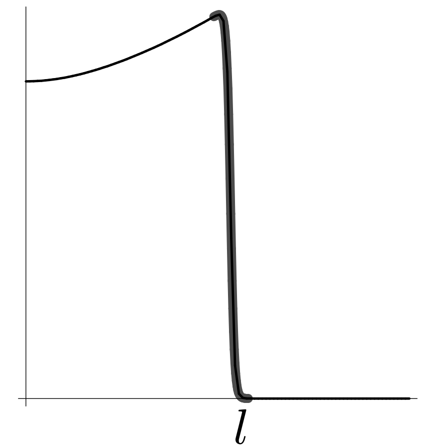
$$w \sim \frac{1}{u} + u \equiv g(u);$$

$$D w_{xx} = \beta_0 g^{-1}(w) - 1$$

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

$$y = \frac{x-l}{\varepsilon};$$

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

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

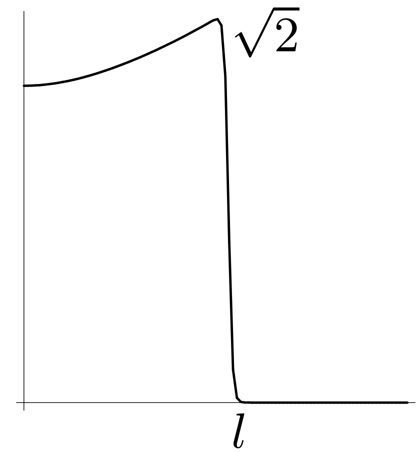
To get a heteroclinic connection the areas between roots of f are equal; obtain

$$w(l) \sim \frac{\sqrt{3}}{2}; \quad u(l^-) \sim \sqrt{2}.$$

Steady state: matching

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

Solve



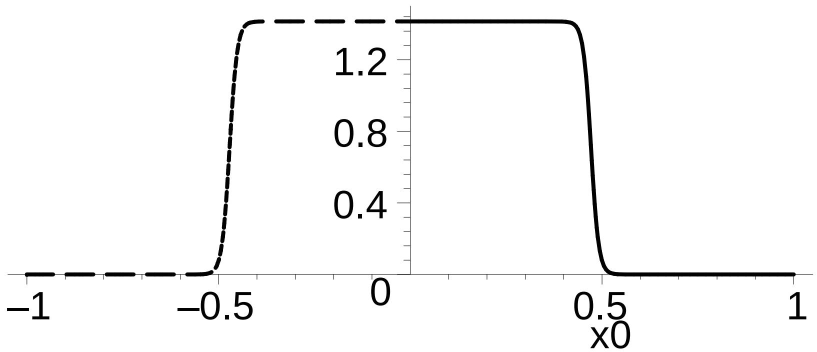
$$\begin{cases} Dw_{xx} = \beta_0 u - 1, \quad x \in (0,l), \\ w = g(u) = \dfrac{1}{u} + u \\ w'(0) = 0, \quad w(l) = g(\sqrt{2}) = \dfrac{3}{\sqrt{2}} \end{cases}$$

and l is determined by

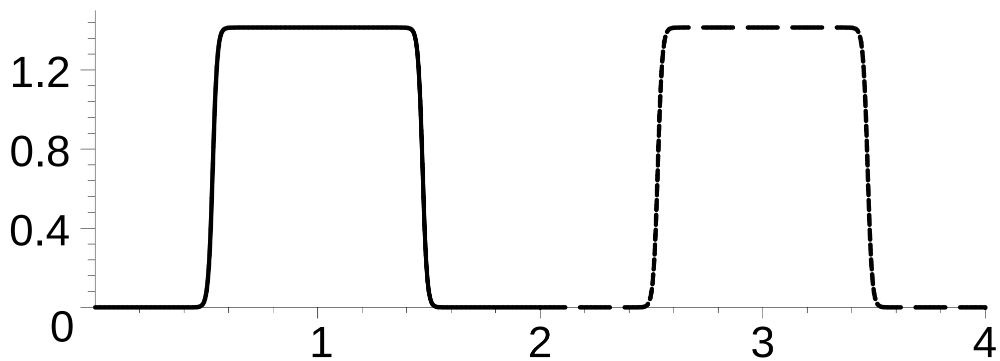
$$\int_0^l u = \frac{L}{\beta_0}.$$

Construction of multiple mesas

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



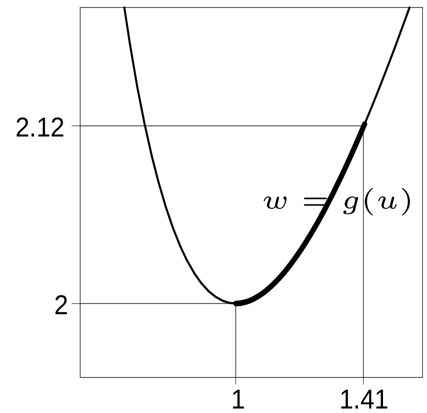
- Replace L by KL and use translation, reflection,



Dissapearence of steady state

- Outer region:

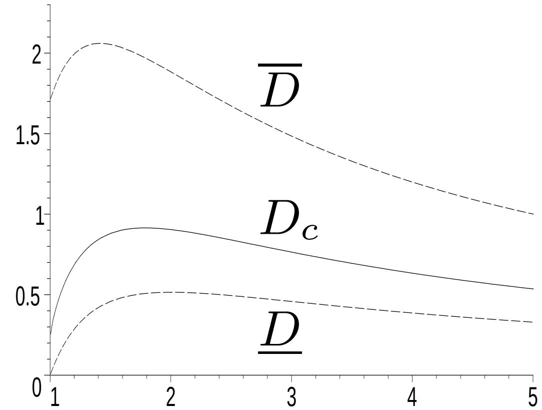
$$\begin{cases} Dw_{xx} = \beta_0 u - 1, \quad x \in (0, l), \\ w = g(u) = \dfrac{1}{u} + u \\ w'(0) = 0, \quad w(l) = g(\sqrt{2}) = \dfrac{3}{\sqrt{2}} \end{cases}$$



- Note that $w(0) \downarrow$ as $D \downarrow$. The min value for $w(0)$ is 2, corresponding to $D = D_c$.

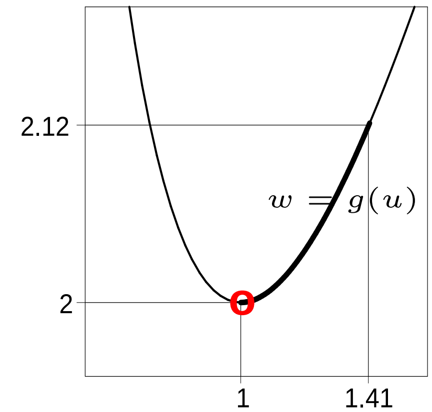
- **Theorem:** Solution exists iff $D > D_c$ where

$$\boxed{\frac{\beta_0 - 1}{4\beta_0^2}(3\sqrt{2} + 4) \leq D_c \leq \frac{\sqrt{2}\beta_0 - 1}{2\beta_0^2}(3\sqrt{2} + 4)}$$

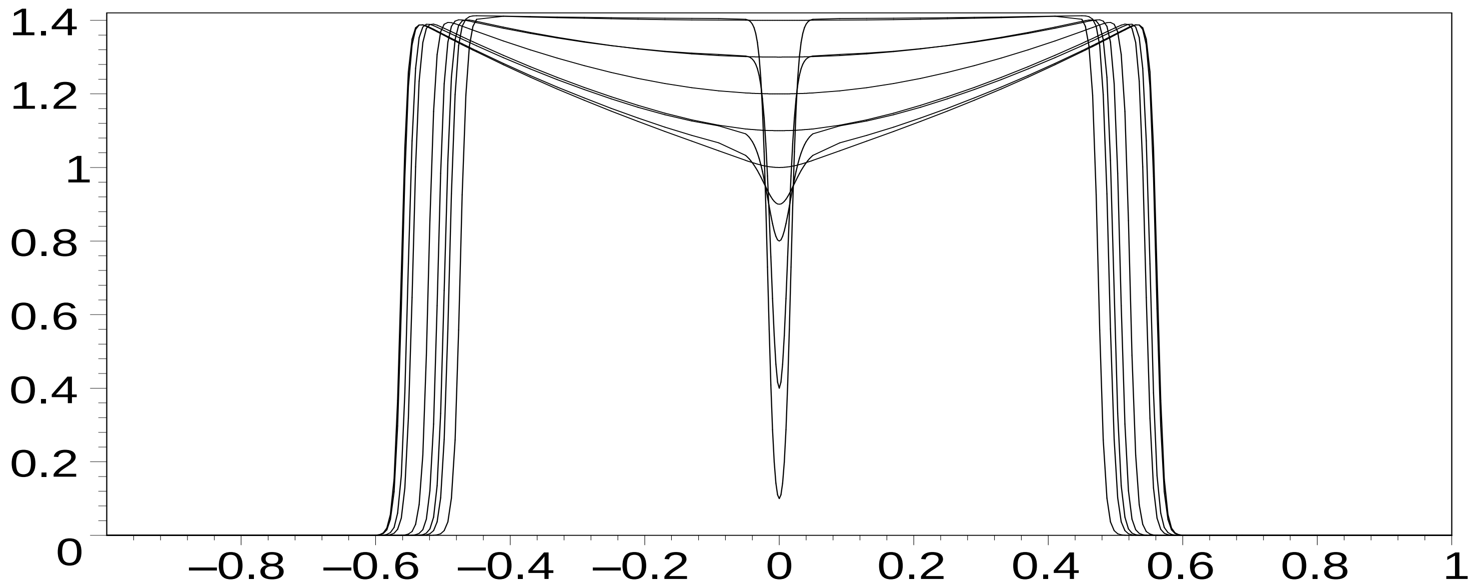


Dissapearence of steady state

- When $D = D_c$, we have asymptotically, $w(0) \sim 2; \;\; u(0) \sim 1.$



- A boundary layer forms near $x = 0$ when D is decreased past D_c:



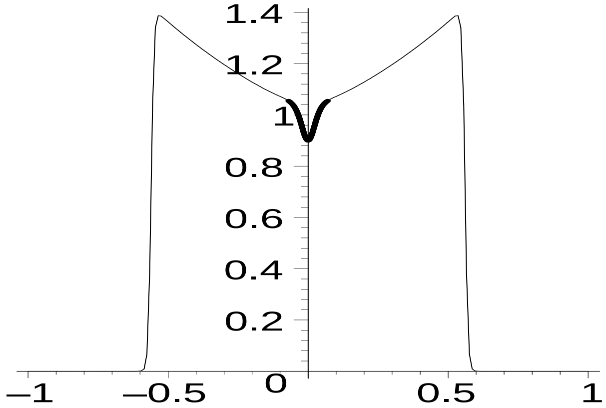
Boundary layer analysis

$$u = 1 + \delta u_1(z) + \cdots ;$$

$$w = 2 + \delta^2 w_1(z) + \cdots ;$$

$$D = D_c + \cdots$$

$$x = z\delta, \quad \delta = \varepsilon^{2/3}$$



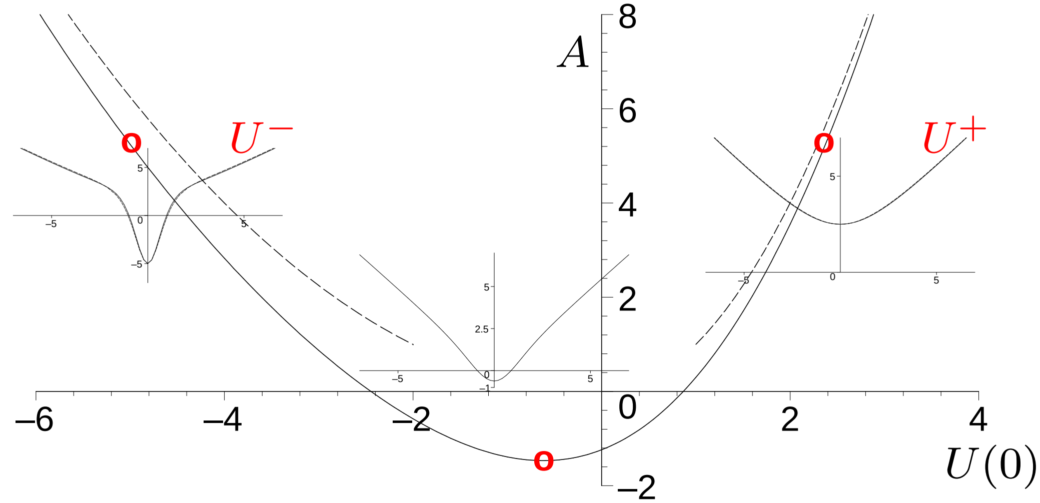
This leads to the core problem

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

with $A = w_1(0)\left(\frac{D_c}{\beta_0 - 1}\right)^{2/3}$.

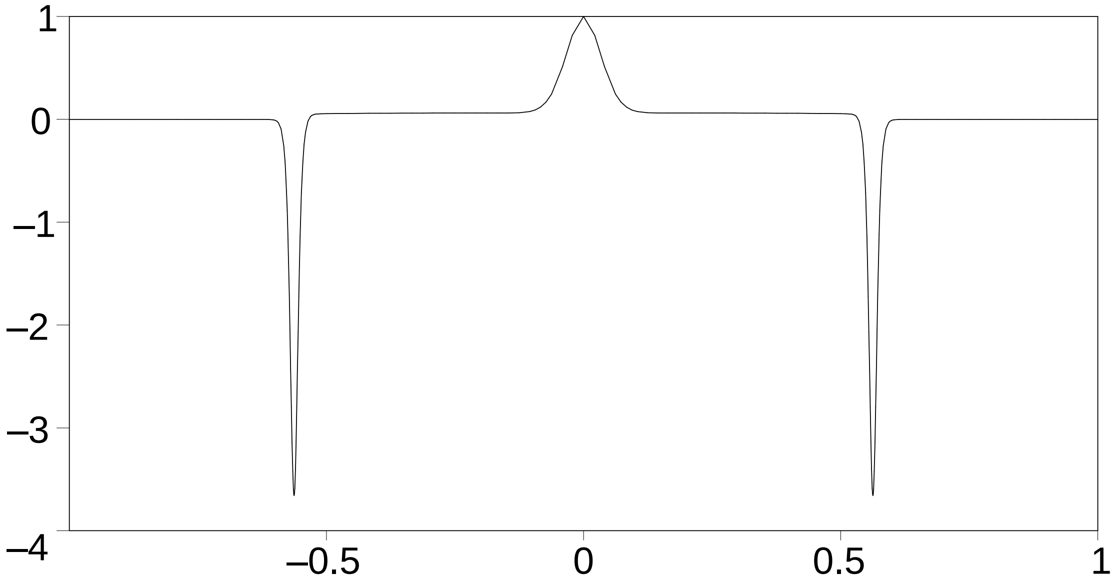
Core problem: $\begin{cases} U''(y) = U^2 - A - y^2; \quad U'(0) = 0 \\ U' \to 1 \text{ as } y \to \infty. \end{cases}$

- When A is large negative then no solutions exists
- When A is large positive there are exactly two *monotone* solutions: $U^+ = \sqrt{A + y^2}; \quad U^- = U^+ \left(1 - 3\,\mathrm{sech}^2\left(\left(\frac{A}{2}\right)^{1/2} y\right)\right).$
- Monotone solution cannot connect to a non-monotone branch: U^+ and U^- connect to each other at $A = A_c$.
- This fold point is *unique*. Self-replication occurs if A is decreased below A_c.



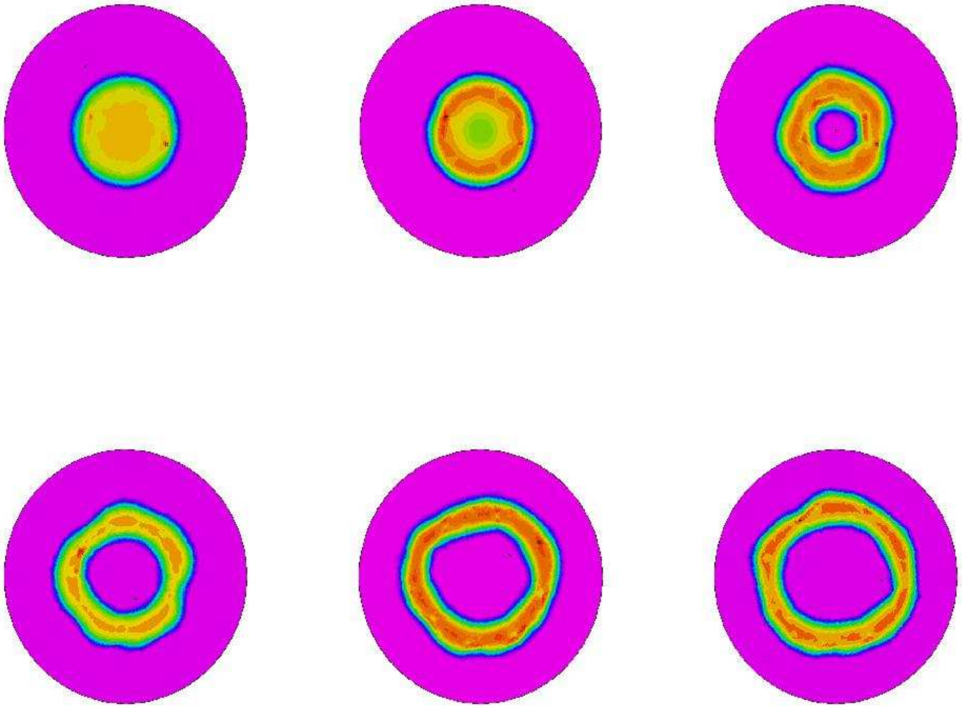
Dimple eigenfunction

At the fold point $A = A_c$, the shape of the eigenfunction is given by $\phi = \frac{\partial U}{\partial A}$. Using monotonicity of U and conservation of mass, we show that the eigenfunction has "dimple" shape, responsible for the initiation of self-replication.



In 2D: “Volcano” instability

$$U''(y) \to U''(r) + \frac{1}{r}U'(r), \quad y^2 \to r^2$$



Universality of the Core Problem

- Some other models that exhibit mesa self-replication are:
  - Keener-Tyson model of BZ reaction:

$$v_t = \varepsilon^2 v_{xx} + v - v^2 - f_0 z \frac{v-q}{v+q}; \quad \tau z_t = D z_{xx} - z + v$$

  - 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:

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

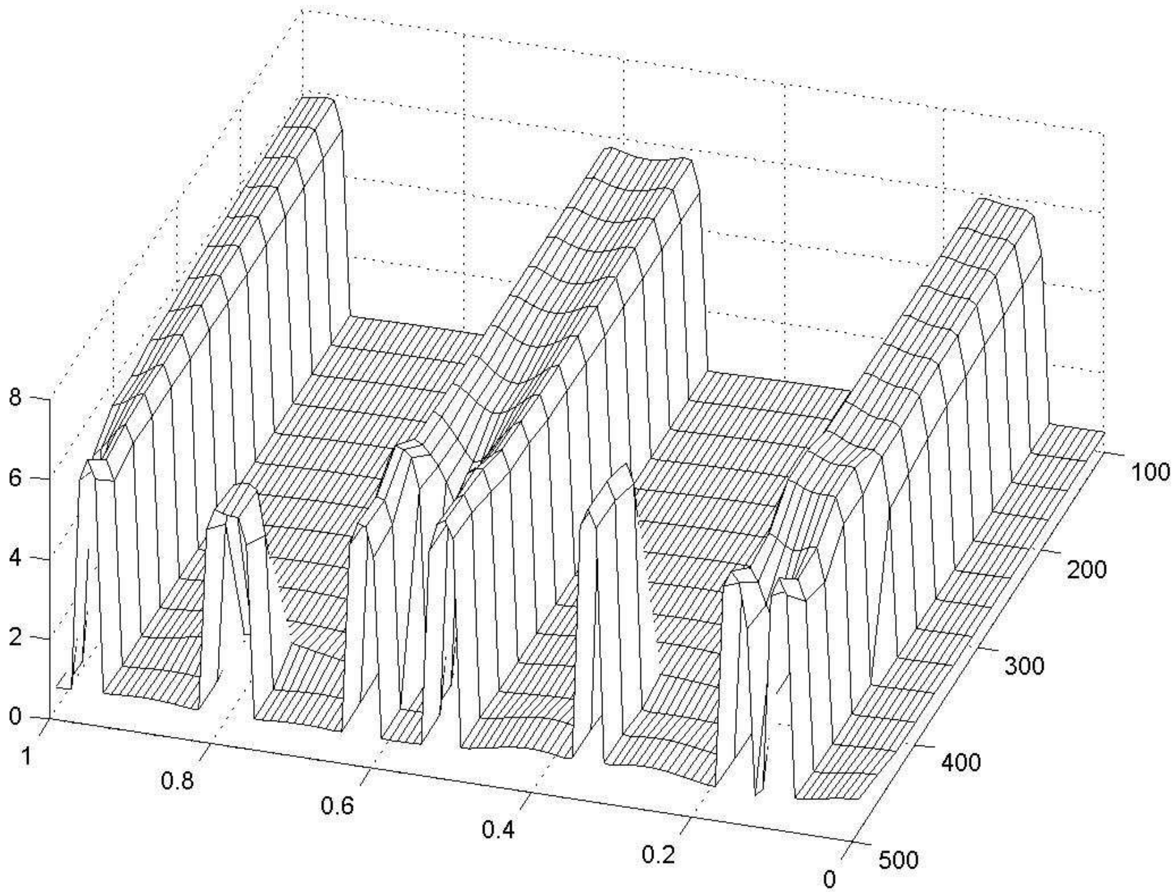
- The same core problem appears at self-replication threshold.

DALHOUSIE UNIVERSITY Inspiring Minds

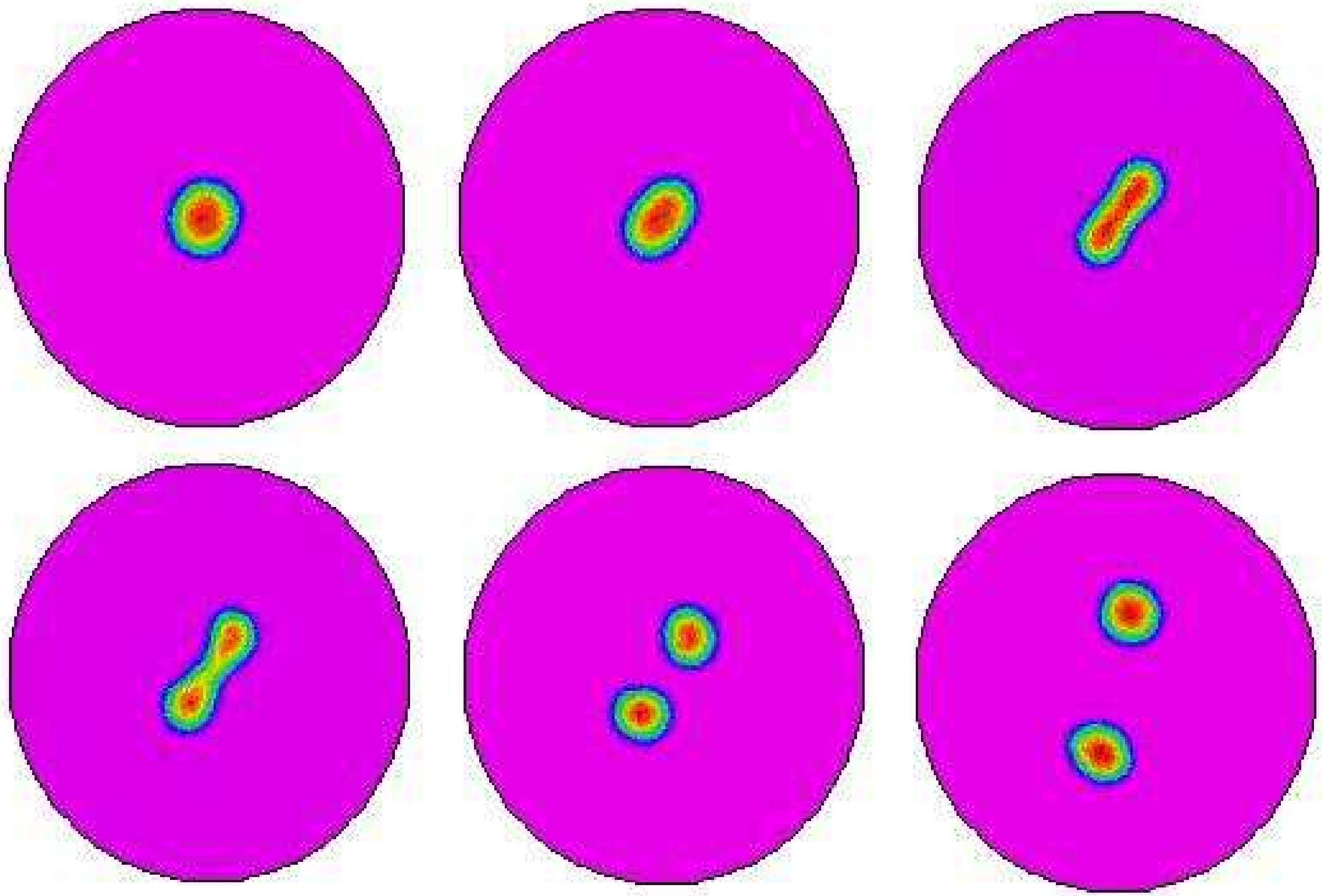
UBC

Universality of the Core Problem

Lengyel-Epstein model:



Part II: Self-replication of spots



Keener-Tyson model of BZ reaction

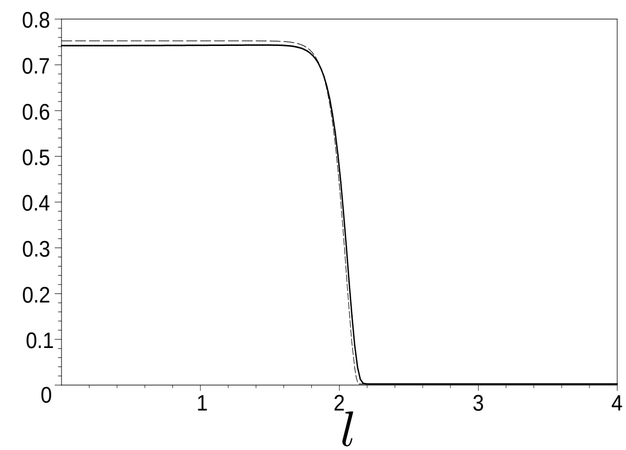
$$v_t = \varepsilon^2 v_{xx} + v - v^2 - f_0 z \frac{v-q}{v+q}; \quad \tau z_t = D z_{xx} - z + v$$

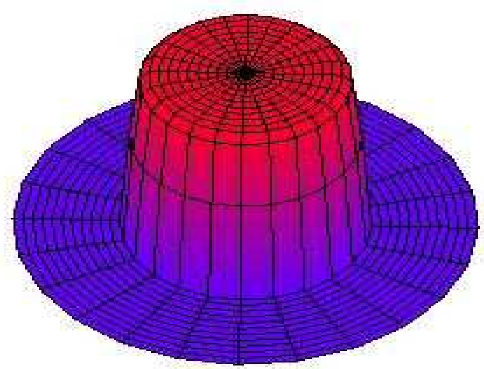
- We assume $\varepsilon \ll 1, \;\; q \ll 1, \tau = 0.$
- Here, we look at the case $D \gg 1$, on a disk of radius R in 2D.
- Radial steady state given by:

$$v \sim \begin{cases} \frac{3}{4} \tanh^2 \left(\frac{r-l}{\varepsilon} 2^{-3/2} \right), & r < l \\ q, & r > l \end{cases};$$

$$z0 \sim \frac{3}{16 f_0};$$

$$l \sim \sqrt{\frac{1}{4 f_0}} R + 2\sqrt{2}\varepsilon$$





Peanut-shaped instability

We consider perturbation of the form:

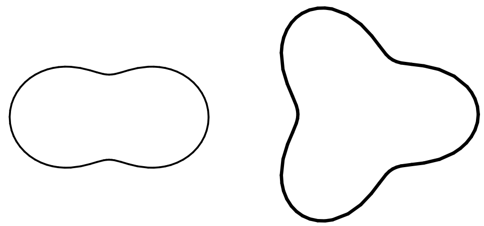
$$v(x,t) = v_e(r) + \exp(\lambda t)\cos(m\theta)\,\phi(r)\,,$$
$$z(x,t) = z_e(r) + \exp(\lambda t)\cos(m\theta)\,\psi(r)$$

and expand $\lambda = \varepsilon\lambda_0 + \ldots$. End result is:

$$\lambda_0 \sim \sqrt{2}\frac{15}{16}\sqrt{f_0}\frac{R}{D}\left(\left(1-\frac{1}{4f_0}\right)-\frac{1}{m}\left(1+\left(\frac{1}{4f_0}\right)^m\right)\right)-\frac{4m^2 f_0\varepsilon}{R^2}.$$

Conclusion: When $f_0 = O(1)$, the radial mesa is

- Unstable in the limit $\frac{\varepsilon}{D} \to 0$
- Stable in the limit $\frac{\varepsilon}{D} \to \infty$
- Instability thresholds when $\frac{\varepsilon}{D} = O(1)$.
- The first unstable mode can be $m = 2$ **or** 3 or...



Spots of “small” radius: $\varepsilon \ll l \ll 1$

Since $l = R/2f_0^{-1/2}$, we get $1 \ll f_0 \ll \frac{1}{\varepsilon^2}$. Then:

$$\lambda_0 = \sqrt{2}\frac{15}{16}\frac{R\sqrt{f_0}}{D}\left(1 - \frac{1}{m} - Am^2\right), \quad A = \frac{64}{15\sqrt{2}}\frac{f_0^{1/2}\varepsilon D}{R^3}$$

- Instability sets in as f_0 is decreased to $f_0 = O\left(\frac{1}{(\varepsilon D)^2}\right)$ and $1 \ll D \ll \frac{1}{\varepsilon}$.
- To solve instability thersholds: $(1 - \frac{1}{m}) - Am^2 = 0, \quad \frac{1}{m^2} - 2Am = 0 \implies m = 3/2, A = 4/27.$
- Conclusion: $m = 2$ is the first unstable mode for “small” spots! The corresponding instability threshold is

$$f_0^{1/2}\varepsilon D R^{-3} = .041.$$

Open questions

- Creation vs. replication
- Core problem in 2D (spot-to-ring): $D = O(1)$
- Interface motion for *large* D (Like Cahn-Hilliard??)
- Spike patterns in the Brusselator and BZ system
- Transition of mesa into a spike ($l = O(\varepsilon)$)
- Dynamics of self-replication in 2D: slowly moving fronts
- Weakly nonlinear analysis?
- Numerical challenges: need very robust code $\varepsilon = 0.005$ to verify the theory of small spots.

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, M.J. Ward, 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