Pattern selection in the wake of fronts

Arnd Scheel, University of Minnesota

[Rothenmund, 1907], [Knöll, 1939]

IMA, 2012

Research supported by NSF
Outline

- Motivation & Models
- Invasion fronts
- Speed and pattern selection
Outline

• Motivation & Models

• Invasion fronts

• Speed and pattern selection
Liesegang patterns in nature and experiment

\[
2\text{NaOH} + \text{MgCl}_2 \rightarrow \text{Mg(OH)}_2
\]
Liesegang patterns in nature and experiment

[George & Varghese]
Liesegang patterns in nature and experiment

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Liesegang patterns in nature and experiment

Lagzi

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Some History

Reaction-diffusion in gels

- Raphael Liesegang (1896)
- Jablzinsky (1923) \( \Delta x_{j+1}/\Delta x_j \rightarrow \eta > 1 \)
- Matalon-Packter (1955):
  \[ \eta \sim g_1([B]) + g_2([B])/[A], g_j \downarrow \]
- **Books:** H.K. Henisch (1988), Crystals in gels and Liesegang rings;
  B.A. Grzybowski (2009), Chemistry in Motion
- **Math:** Keller & Rubinow (1981), Hilhorst, vd Hout, Mimura, Ohnishi (2007,2009)
Reaction-Diffusion Models

Outer and inner electrolyte $A, B$; product $C$ solute, $E$ precipitate.

$$A + B \rightarrow C, \quad C \rightleftharpoons E$$

Models on $x \in \mathbb{R}_+$

$$a_t = d_a \Delta a - ab$$

$$b_t = d_b \Delta b - ab$$

$$c_t = d_c \Delta c - f(c, e) + ab$$

$$e_t = d_e \Delta e + f(c, e)$$

$$f(c, e) = e(1 - e)(e - a) + \gamma c$$

Initial and boundary conditions

$$t = 0 : b \equiv b_0 > 0, \ a, c, e \equiv 0 \quad \text{b.c.} : a|_{x=0} = a_0 \& \text{Neumann}$$
Reaction-Diffusion Models

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Precipitation: super-saturation vs Cahn-Hilliard

Super-saturation

\[ c_t = c_{xx} - f(c, e) + ab \]

\[ e_t = d e c_{xx} + f(c, e) \]

[Ostwald 1897, Keller & Rubinow ’81]

Problems:

• not smooth, no width law
• numerically subtle
• no exotic patterns
• not structurally stable
Precipitation: super-saturation vs Cahn-Hilliard

Super-saturation
\[ c_t = c_{xx} - f(c, e) + ab \]
\[ e_t = d_e c_{xx} + f(c, e) \]

[Cahn-Hilliard 1897, Keller & Rubinow '81]

Cahn-Hilliard
\[ u \sim e/(c + e) \in [0, 1] \]
\[ u_t = -\Delta (d\Delta u + g(u)) + ab \]

[Cahn & Hilliard '58, Droz 90's]

• Phenomenological model for nucleation and growth
• limit of threshold kinetics description \( \gamma \to \infty \)

Problems:
• not smooth, no width law
• numerically subtle
• no exotic patterns
• not structurally stable

Problems:
• only phenomenological
• no quantitative comparisons
• no exotic patterns
• only one length scale, no \( d_c \)
Chemotaxis

$u$ bacteria, $v$ chemoattractant — Keller-Segel:

\[
    u_t = u_{xx} - (uv_x)_x
\]
\[
    v_t = \kappa v_{xx} - v + u
\]

Instability for high concentrations:

Collective aggregation

w/ M Holzer; REU Students K Bose, T Cox, S Silvestri, P Varin
Chemotaxis

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Instability for high concentrations:

Collective aggregation versus ripening

w/ M Holzer; REU Students K Bose, T Cox, S Silvestri, P Varin
More timely: Opinion dynamics

Opinion dynamics: $x$ opinion, $u$ people, $v$ money

$$u_t = u_{xx}$$

$$v_t = \kappa v_{xx} - v$$

People communicate and spend,
More timely: Opinion dynamics

Opinion dynamics: $x$ opinion, $u$ people, $v$ money

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People communicate and spend, people make money
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Instability when there’s too much money:

Compromise
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\[ v_t = \kappa v_{xx} - v + u \]

People communicate and spend, people make money, money attracts opinion…

Instability when there’s too much money:

Compromise versus winner-takes-all
Different: surface-roughening and ion beams

- Surface bombardment with ion beams $\rightarrow$ instabilities
- Surface roughness on nano-scales;
- Highly disordered structure
- But masked fronts create highly organized surface ripples, nano-dots, ...

[Gelfand&Bradley]
Pattern formation: fronts versus noise

\[
\begin{align*}
    c_t &= \Delta c - e(1 - e)(e - a) - \gamma c \\
    e_t &= e(1 - e)(e - a) + \gamma c
\end{align*}
\]

Linear Stability of equilibria

Perturbing \( e = a, c = 0 \) random amplitudes

random locations

w/ Qiliang Wu, REU students M Kotzagiannidis, J Peterson, J Redford
Invasion fronts: free and triggered

Spatio-temporal source term \( h(t, x) \), depositing mass

\[
\begin{align*}
  c_t &= \Delta c - f(c, e) + h(t, x) \\
  e_t &= \kappa \Delta e + f(c, e)
\end{align*}
\]

Basic example: \( h(t, x) = H(x - st) \), \( H \) localized

Fast source \( s \sim 1 \)

Slow source \( s \ll 1 \)
Invasion fronts: free and triggered

Spatio-temporal source term $h(t, x)$, depositing mass

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Basic example: $h(t, x) = H(x - st)$, $H$ localized

**Fast source** $s \sim 1$ \hspace{2cm} **Slow source** $s \ll 1$
Multi-dimensional patterns

A plethora of patterns from “growth” and “threshold conversion”:

Wet stamping — isotropic

— anisotropic

trigger front and inhomogeneity
Multi-dimensional patterns

A plethora of patterns from “growth” and “threshold conversion”:

Wet stamping — isotropic — anisotropic

trigger front and inhomogeneity
Outline

• Motivation & Models
• Invasion fronts
• Speed and pattern selection
Existence of invasion fronts

Two approaches:

**Robustness:**
Show that linearization at a given front is Fredholm index 0 — without proving existence!

**Existence:**
Show that fronts exist using Conley’s index!
Robustness — phenomena

Initial conditions \((c \equiv 0, \ e \equiv a)\) + perturbation near \(x = 0\)

\[
\begin{align*}
\gamma &= 0.001, \ a = 0.04 & \gamma &= 0.001, \ a = 0.4 & \gamma &= 1.5, \ a = 0.22
\end{align*}
\]

- **Bulk Front**
- **Transient Pattern**
- **Persistent Pattern**

\[
\begin{align*}
\frac{ct}{c} &= c_{xx} - e(1-e)(e-a) - \gamma c \\
\frac{et}{e} &= de_{xx} + e(1-e)(e-a) + \gamma c
\end{align*}
\]
Robustness — results

**Theorem** [R Goh, S Mesuro, S.]

Pattern-forming fronts are robust iff the pattern in the wake is stable with respect to co-periodic perturbations

**Remarks**

- Effectively discriminate between transient and persistent patterns!
- All periodic patterns are unstable on $x \in \mathbb{R}$ or period 2!
- Bulk fronts are pushed fronts; [van Saarloos]
- The transition from bulk to pattern-forming is an “essential, pointwise” Hopf bifurcation at $a_*(d)\ldots$
Robustness — proofs

- Traveling-wave equation for \( u = (c, e)(x - st, kx) \) as dyn’ sys’
  
  \[
  \begin{align*}
  u_\xi &= -k \partial_y u + v \\
  v_\xi &= -k \partial_y v - D^{-1} (F(u) + c(v - k \partial_y u))
  \end{align*}
  \]
Robustness — proofs

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• Invasion fronts \( \iff \) Heteroclinic orbits \( u^-(y) \rightarrow u^+(y) \) (but ill-posed!)
Robustness — proofs

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• Invasion fronts $\iff$ Heteroclinic orbits $u_-(y) \rightarrow u_+(y)$ (but ill-posed!)

• Robustness $\iff$ transverse intersections $W^s_+ \cap W^-_u$
Robustness — proofs

- Traveling-wave equation for $u = (c, e)(x - st, kx)$ as dyn’ sys’
  
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- Invasion fronts $\iff$ Heteroclinic orbits $u^-(y) \longrightarrow u^+(y)$ (but ill-posed!)

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- Ill-posed, pseudo-elliptic: relative Morse indices!
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• Traveling-wave equation for \( u = (c, e)(x - st, kx) \) as dyn' sys' 
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  \]

• Invasion fronts \iff Heteroclinic orbits \( u_*(y) \rightarrow u_*^+(y) \) (but ill-posed!)

• Robustness \iff transverse intersections \( W^s_+ \cap W^-_u \)

• Ill-posed, pseudo-elliptic: relative Morse indices!

**Linearize** at \( u^+_\pm(y) \) and count dimension of \( W^s_+, W^-_u \):

\[
\iota : (u_+ \in TW^s_+, u_- \in TW^-_u) \mapsto u_+ - u_-
\]

**Index theorem** e.g. [Sandstede,S. '01]: Fredholm = relative Morse:

\[
i_F(\iota) = i_M(u^-_*) - i_M(u^+_*)
\]
Resonant modes and Morse indices

How do we compute $i_M(u_\pm)$? \(\rightarrow\) Homotopies!

Spatial growth modes $u(y)e^{\nu \xi}$ satisfy

$$-s\nu u = D(k\partial_y + \nu)^2u + F'(u_{\star})u$$

Idea: Homotope $u_{\star} = u_{\star}^- \ldots u_{\star}^+$ and count $\nu$'s crossing $\mathbb{R}$
Resonant modes and Morse indices

How do we compute $i_M(u^\pm_*)$? \[\rightarrow\] Homotopies!

Spatial growth modes $u(y)e^{\nu \xi}$ satisfy

$$-s\nu u = D(k\partial_y + \nu)^2u + F'(u_*)u$$

Idea: Homotope $u_* = u^-_* \ldots u^+_*$ and count $\nu$'s crossing $i\mathbb{R}$

Here's how: homotope to $\lambda = +\infty$ for $u_* = u^\pm_*$:

$$\lambda u - s\nu u = D(k\partial_y + \nu)^2u + F'(u_*)u$$

where we can neglect $F'$ and hence the dependence on $u$:

Crossings in $\lambda$ $\iff$ resonant unstable modes
### Existence: The Cahn-Hilliard equation

A model for phase separation, \( u \) order parameter

\[
    u_t = -(u_{xx} + u - u^3)_{xx}
\]

on \( \mathbb{R}/L\mathbb{Z} \), say

**Mass conservation**

\[
    m(u) = \int u
\]

**Energy dissipation**

\[
    E(u) = \int u_x^2 - u^2 + \frac{1}{2} u^4
\]

**Gradient structure**

\[
    u_t = -\nabla_{H^{-1}} E(u)
\]
Equilibria and attractors

Dynamics on attractor: equilibria and heteroclinic connections

\[
|m| < \frac{1}{\sqrt{5}}
\]

\[
\frac{1}{\sqrt{5}} < |m| < \frac{1}{\sqrt{3}}
\]

\[
\frac{1}{\sqrt{3}} < |m| < 1
\]

[Grinfeld, Novick-Cohen]
Spinodal decomposition fronts

Main Theorem [S.]

For each $|m| < 1/\sqrt{3}$, there exists a modulated front solution

$$u_*(x - s_{\text{lin}}t, k_{\text{lin}}x), \quad u_*(\xi, y) = u_*(\xi, y + 2\pi)$$

with asymptotics

$$\begin{cases} 
  u_*(\xi, y) \to m, & \xi \to +\infty, \text{ unif. in } y, \\
  u_*(\xi, y) \to u_-, & \xi \to -\infty, \text{ unif. in } y,
\end{cases}$$

More specifically,

- For $|m| < 1/\sqrt{5}$, $u_-$ has minimal period $2\pi/k_{\text{lin}}$.

- For $1/\sqrt{5} < |m| < 1/\sqrt{3}$, exist chain of waves $u_{*,1}, \ldots, u_{*,j}$ so that the last wave connects to $u_-,j$ with minimal period $2\pi/k_{\text{lin}}$. 
"Translate" Lyapunov function $\mathcal{L}$ and mass conservation $\mathcal{I}$:

$$
\mathcal{L}(u) = \int_0^{2\pi} \left( \frac{1}{2} u_\xi^2 - G(u) - ku_\xi u_\tau - \frac{1}{s} \theta \theta_\xi \right) d\tau
$$

$$
\mathcal{I}(u) = \int (su - \theta_\xi)
$$

with $G'(u) = u - u^3$, $\theta = u_\xi + G'(u)$
Existence — Outline

• "Translate" Lyapunov function $\mathcal{L}$ and mass conservation $\mathcal{I}$:

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with $G'(u) = u - u^3$, $\theta = u_\xi \xi + G'(u)$

• $H^{-1}$-estimates: define $\partial_{\tau} \phi = u - \int_{\tau} u$!

$$\int_{\xi} \int_{\tau} (\phi^2_{\xi\xi} + \phi^4_\xi) \chi(\xi) < \infty, \quad \int_{\xi} \left( \int_{\tau} su - \mathcal{I} \right)^2 < \infty$$
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• Galerkin approximations in $\tau$, a priori estimates, give Conley index of bounded solutions as isolated invariant set
Existence — Outline

- "Translate" Lyapunov function $\mathcal{L}$ and mass conservation $\mathcal{I}$:

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\int_\xi \left(\int_\tau su - \mathcal{I}\right)^2 < \infty
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- Galerkin approximations in $\tau$, a priori estimates, give Conley index of bounded solutions as isolated invariant set

- Morse indices and connection matrices [Franzosa],[Mischaikow]

→ heteroclinic orbits
Outline

• Motivation & Models

• Invasion fronts

• Speed and pattern selection
Spreading speeds

Absolute and convective instabilities: $u_0(x)$ compactly supported

pointwise growth  pointwise decay  spreading speed

Linear dispersion relation

$u = (c, e) \sim (c_0, e_0) e^{\lambda t + \nu x}$,

$D(\lambda, \nu) = 0$

Pointwise growth modes $(\lambda, \nu)$:

$D(\lambda, \nu) = 0$,

$\partial_\nu D(\lambda, \nu) = 0$ + “pinching”

Classic "Lemma": Typically,

pointwise instability $\iff$ unstable pointwise modes, $\text{Re } \lambda > 0$

Pointwise spreading speed:

$s_{pt} := \sup \{ s | \text{ pointwise unstable in frame } \xi = x - st \}$

Selected wavenumber:

$k_{lin} = \omega_{lin} / s_{pt}$ where $i\omega_{lin}$ neutral pointwise growth mode at
Spreading speeds — subtleties

The previous slide often gives the wrong answer [w/ M Holzer]:

- Linear speeds $< \llap{\text{“pinched speed”}}$

\[
\begin{align*}
    u_t &= u_x + u, \\
    v_t &= -v_x + v
\end{align*}
\]

has pointwise decay, yet a pinched double root at $\lambda = 1$

- Linear speed $< \llap{\text{nonlinear speed: \rightarrow pushed fronts}}$

\[
\begin{align*}
    u_t &= u_{xx} + u(1 - u)(u - a), \\
    a &< 1/3
\end{align*}
\]

- Nonlinear speed $< \llap{\text{linear speed \rightarrow Lotka-Volterra}}$

- Linear speed $< \llap{\text{nonlinear speed: \rightarrow staged invasion}}$

Related question: What happens in the wake of invasion?
Spreading speeds — multi-d

Consider isotropic system, initial conditions $u_{cpt}(x)e^{iky}$.
Define transverse modulated spreading speeds $s_{\text{lin}}(k)$

Conjecture... Theorem? [R Goh, M Holzer, S.]

$s_{\text{lin}}(k) \leq s_{\text{lin}}(0)$

Linear theory *always* predicts stripes in the leading edge of invasion fronts

Other patterns emerge through pushed fronts or staged invasion:

Cahn-Hilliard in strip
Coupled KPP

Toy model for staged invasion

\[ u_t = u_{xx} + u(1 - u) \]

\[ v_t = dv_{xx} + g(u)v - v^3 \]

How do compactly supported initial data evolve?

- **u-equation**: convergence to critical KPP front \( s_u = 2 \)

- **v-equation**: speeds
  - \( u = 0 \): \( s_v = 2 \sqrt{dg(0)} \)
  - \( u = 1 \): \( s_v = 2 \sqrt{dg(1)} \)

**Question**: Determine the \( v \)-invasion speed!
Coupled KPP — phenomena

\[ u_t = u_{xx} + u(1 - u) \]

\[ v_t = dv_{xx} + g(u)v - v^3 \]

“Instantaneous” \( v \)-speed:

\[ s_v = -2 \sqrt{d g(u)} \]

E.g. \( g(u) = 0.3 + a_1 u - 3u^2 \)

3 Regimes:
- locked regime (strong inhomogeneity)
- accelerated regime (intermediate)
- pulled regime (weak, uncoupled)
Resonance poles, locked, and accelerated fronts

Linearizing $v$-equation along $u$-front gives

$$v_t = d v_\xi \xi + 2 v_\xi + g'(u_{KPP}) v = \mathcal{L}u$$

Resonance pole $\lambda_{rp}$ of $\mathcal{L}$ determine regime:

- $\lambda_{rp} > 0 \implies$ locked fronts, $s_v = 2$
- $0 > \lambda_{rp} > -\lambda_* \implies$ accelerated fronts, $s_v > s_v^1 = \sqrt{dg(1)}$

Acceleration since resonance mode induces spreading:

$$v(\xi) \sim e^{\lambda_{rp} t + \nu_+} \text{ for } \xi \to +\infty, s_v = \lambda/\nu_+$$

Note:

$u$-front accelerates $v$-front by fixed amount while separation distance goes to infinity!

Interaction force growing exponentially with distance
Accelerated fronts — proofs

Idea:
Construct steep sub- and supersolutions based on the resonance pole

Similar technique: [Nolen, Roquejoffre, Ryzhik, Zlatos 2012] → KPP with steady inhomogeneity, compact support

\[ u_t = u_{xx} + g(x)u - u^2 \]
Locked fronts

Theorem
Suppose $\lambda_{rp} > 0$, then there exists stable locked front, $v$-component has steep exponential decay

$$u = u_{kpp}(x - 2t), \ v_{lock}(x - 2t) \sim e^{-d^{-1}(1 + \sqrt{1 + dg(1)})}\xi$$

For $\lambda_{rp} > 0$, small, the bifurcation to locked fronts is supercritical and the separation distance scales with

$$\frac{1}{2\nu_v^+} \log(\lambda_{rp}) \text{ if } 2\nu_v^+ - \nu_v^- > 0$$

$$\frac{1}{\nu_v^-\nu_v^+} \log(\lambda_{rp}) \text{ if } 2\nu_v^+ - \nu_v^- < 0$$

Proof Heteroclinic orbit flip, Shilnikov coordinates after normal form transformations that straighten fibrations [Homburg].
Comparison with simulations

Fix \( g(u) = 0.3 + \alpha(u - u^2), \ d = 1. \)

Speed versus prediction
locked, accelerated, uncoupled

Separation versus prediction, locked case
Summary and references

Pattern-forming fronts need more attention!

• existence and robustness
• speeds and wavenumber predictions — 1-d
• some results for multi-d, staged invasion

References

• existence & robustness:
  A Scheel, *Spinodal decomposition and coarsening fronts in the Cahn-Hilliard equation*, very soon

• staged invasion and anomalous spreading: M Holzer, A Scheel,
  *A slow pushed front in a Lotka-Volterra competition model*, Nonlinearity 2012
  *Accelerated fronts in a two stage invasion process*, preprint