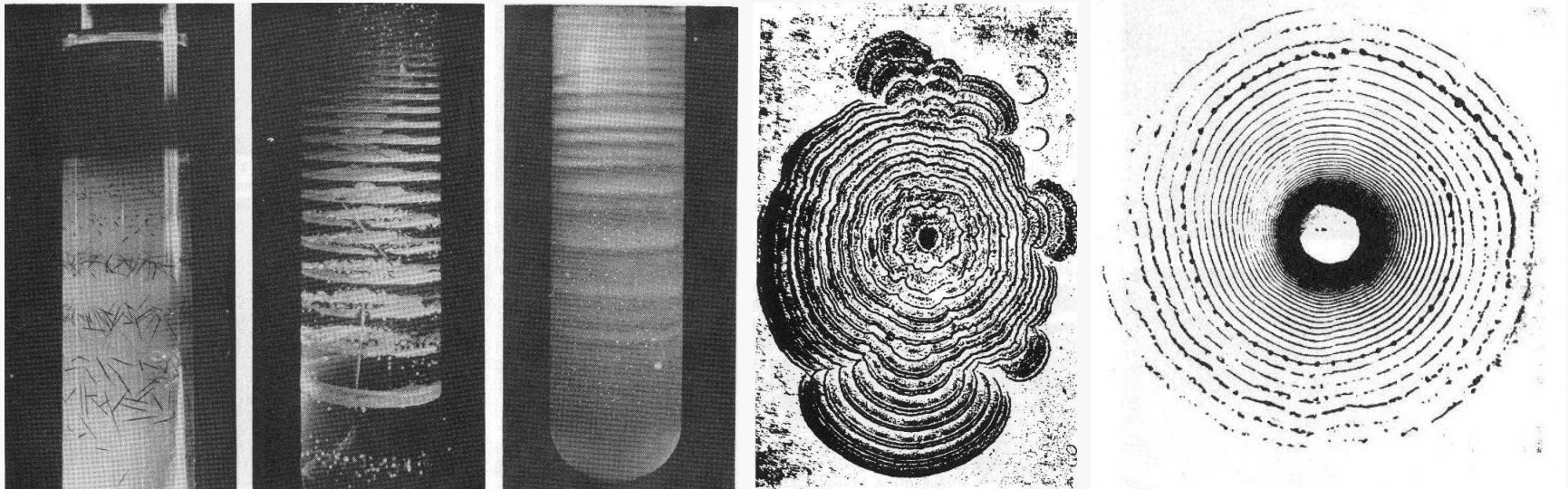


Pattern selection in the wake of fronts

Arnd Scheel, University of Minnesota



[Rothmund,1907],[Knöll,1939]

IMA, 2012

Research supported by NSF

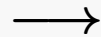
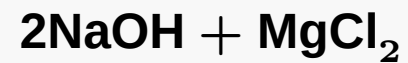
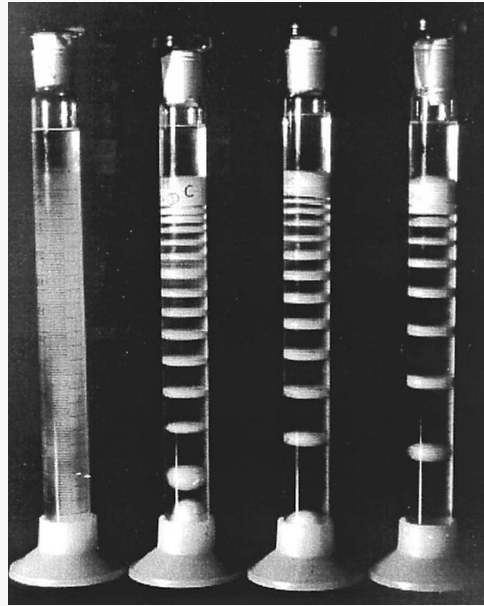
Outline

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

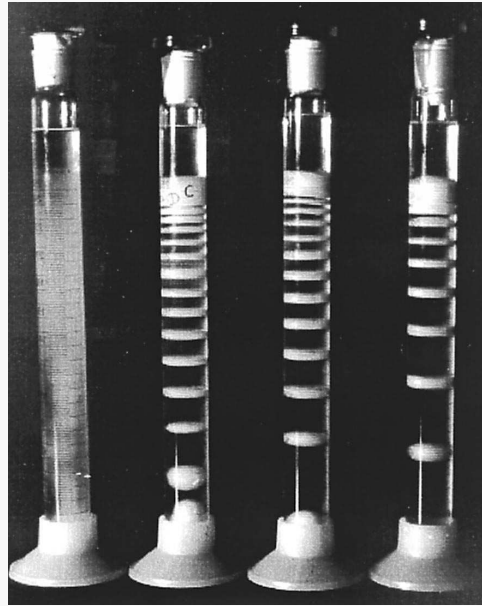
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Liesegang patterns in nature and experiment



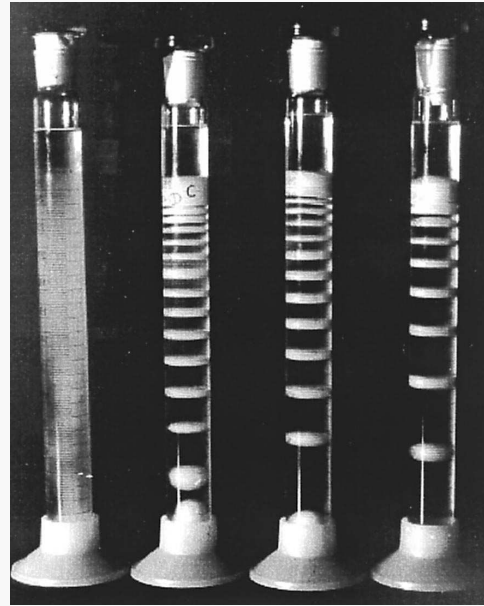
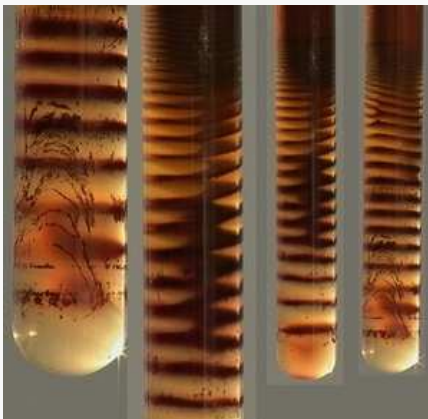
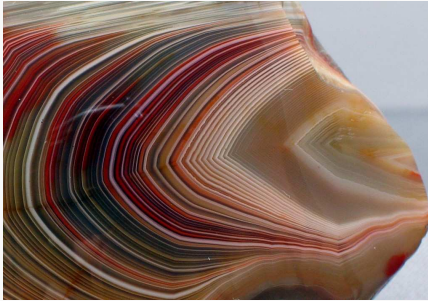
Liesegang patterns in nature and experiment



Gel	B	A
Agar	Zn^{2+}	OH^-
Agar	Fe^{2+}	NH_3
Agar	I^-	Pb^{2+}
Agar	F^-	Pb^{2+}
Agar	Mn^{2+}	S^{2-}
Agar	Cu^{2+}	S^{2-}
Agar	Cd^{2+}	S^{2-}
Agarose	Al^{3+}	OH^-
Gelatin	Ba^{2+}	SO_4^{2-}
Gelatin	Co^{2+}	NH_3
Gelatin	Ni^{2+}	NH_3
Gelatin	$\text{Cr}_2\text{O}_7^{2-}$	Ag^+
Gelatin	$\text{Cr}_2\text{O}_7^{2-}$	Pb^{2+}
Gelatin	OH^-	Mg^{2+}
Gelatin	Co^{2+}	OH^-
Gelatin	Ni^{2+}	NH_3
Gelatin	Cd^{2+}	NH_3
Gelatin	Mg^{2+}	NH_3
Silica	HPO_4^{2-}	Ca^{2+}
Poly(vinyl alcohol)	Cu^{2+}	OH^-
Poly(vinyl alcohol)	Co^{3+}	OH^-

[George&Varghese]

Liesegang patterns in nature and experiment

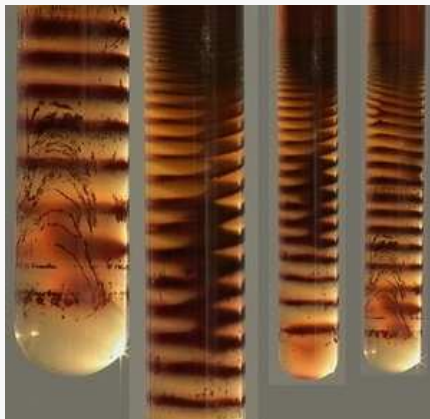
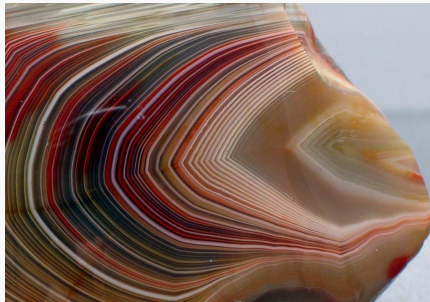


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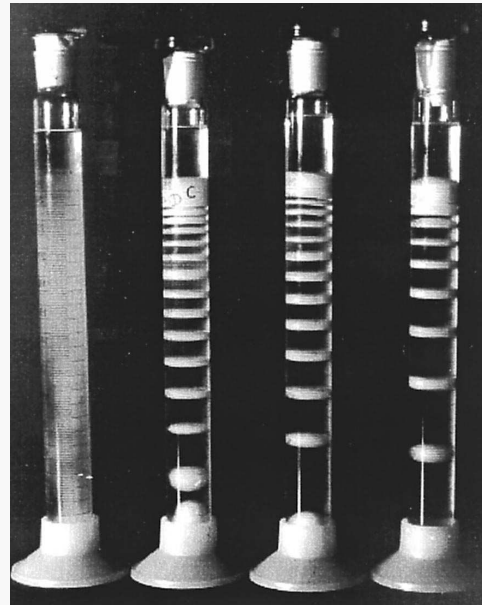
[Lagzi]

[George&Varghese]

Liesegang patterns in nature and experiment

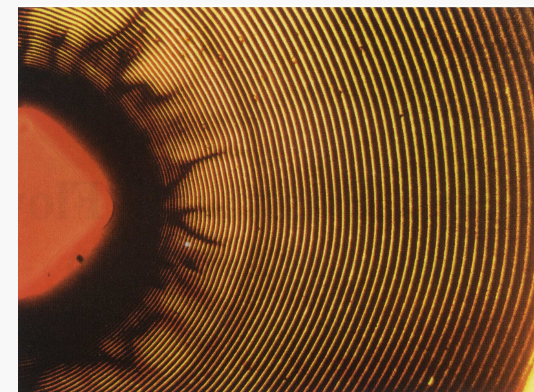
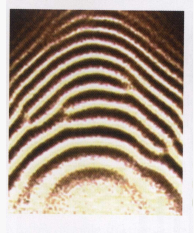
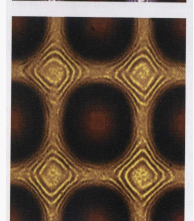
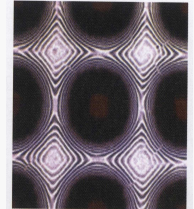
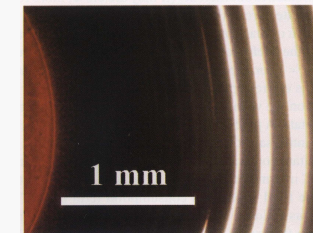
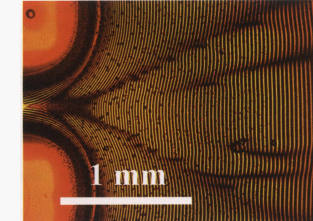
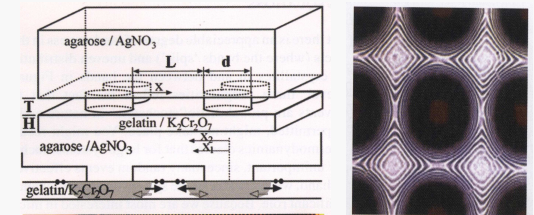


[Lagzi]



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[George&Varghese]



[Grzybowski]

Some History

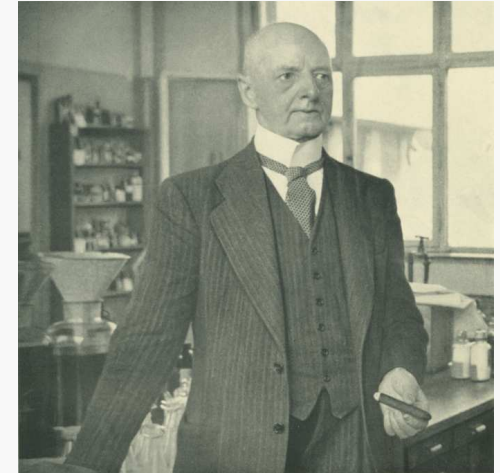
Reaction-diffusion in gels

- **Raphael Liesegang (1896)**
- **Jablzinsky (1923)** $\Delta x_{j+1} / \Delta x_j \rightarrow \eta > 1$
- **Matalon-Packter (1955):**

$$\eta \sim g_1([B]) + g_2([B])/[A], g_j \searrow$$

- **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.



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

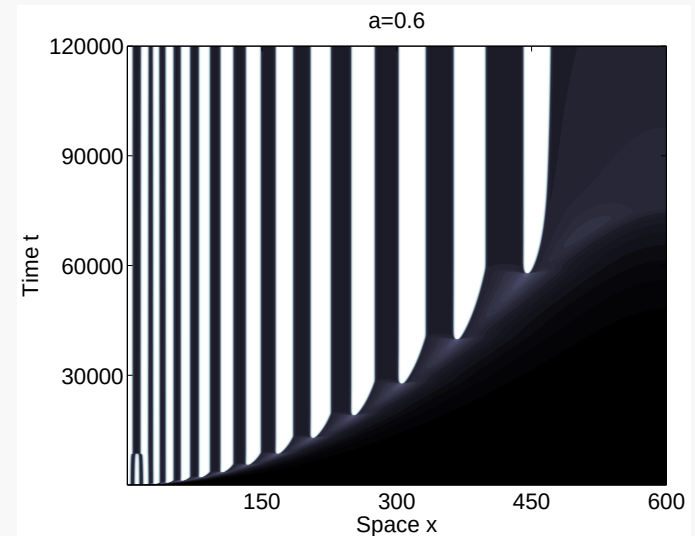
$$a_t = d_a \Delta a - ab$$

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

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

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



w/ R Goh, S Mesuro, REU

Initial and boundary conditions

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

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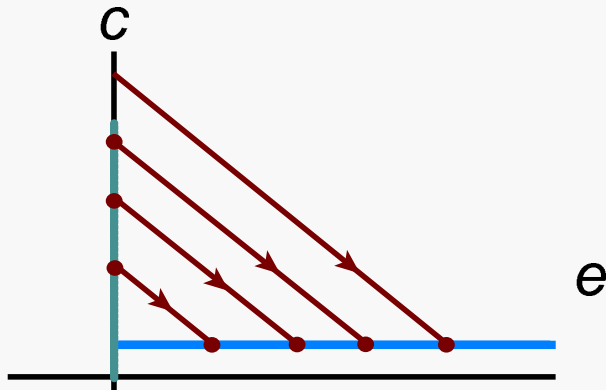
Precipitation: super-saturation vs Cahn-Hilliard

Super-saturation

$$c_t = c_{xx} - f(c, e) + ab$$

$$e_t = \cancel{d_e c_{xx}} + f(c, e)$$

[Ostwald 1897, Keller&Rubinow '81]



Problems:

- not smooth, no width law
- numerically subtle
- no exotic patterns
- not structurally stable

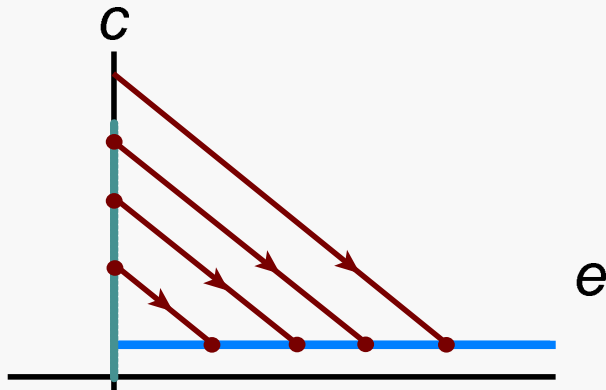
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[Ostwald 1897, Keller&Rubinow '81]



Problems:

- not smooth, no width law
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- **not structurally stable**

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 $\gamma \rightarrow \infty$

Problems:

- only phenomenological
- no quantitative comparisons
- no exotic patterns
- only one length scale, no d_c

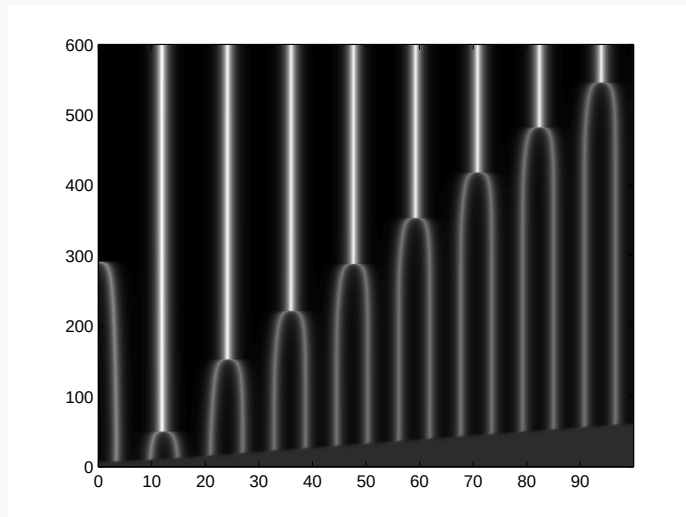
Chemotaxis

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

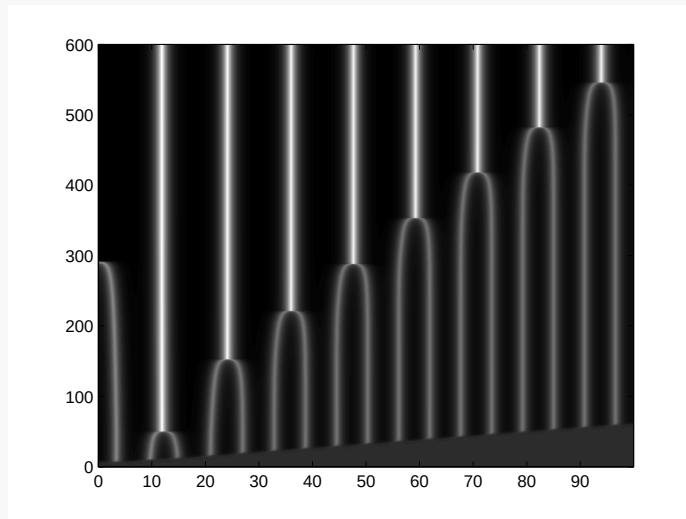
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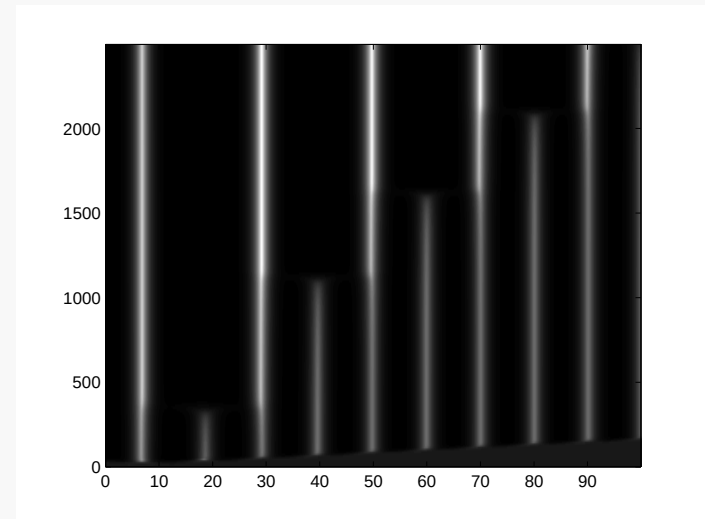
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Instability for high concentrations:



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

$$u_t = u_{xx}$$

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

People communicate and spend, people make money

More timely: Opinion dynamics

Opinion dynamics: x opinion, u people, v money

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

More timely: Opinion dynamics

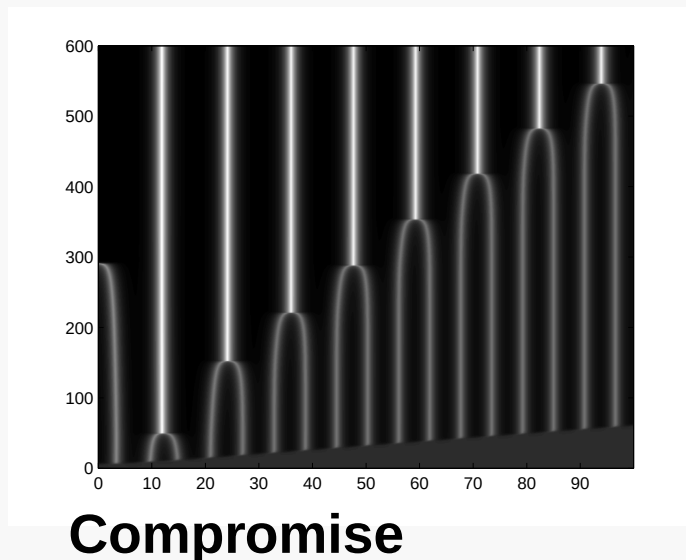
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Instability when there's too much money:



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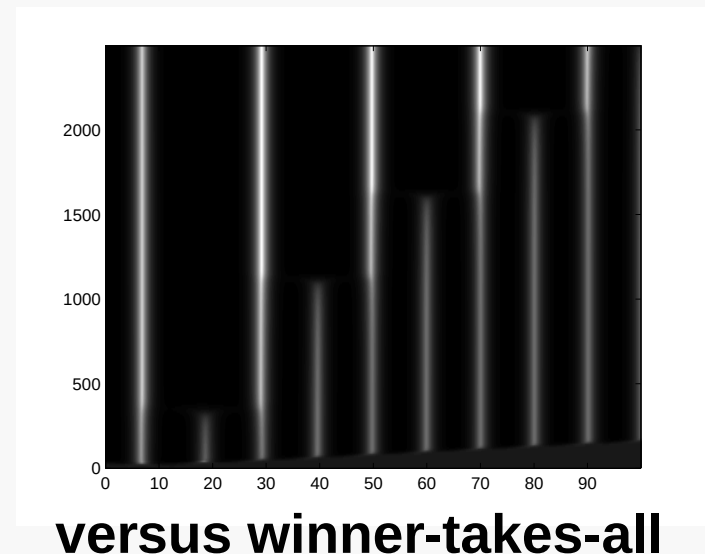
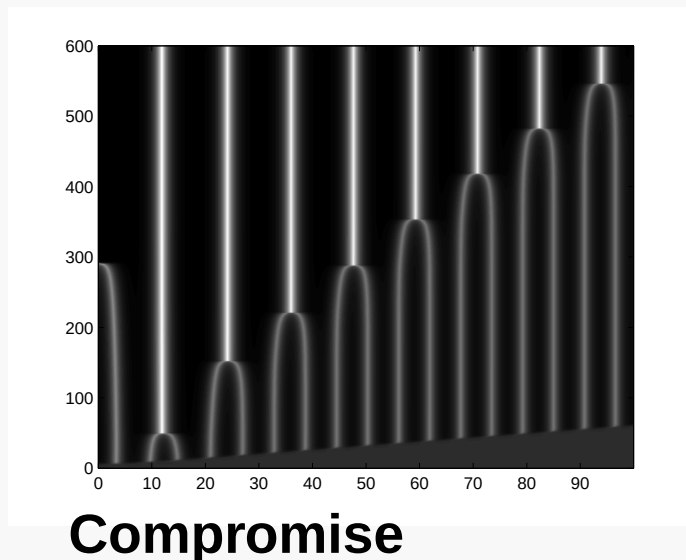
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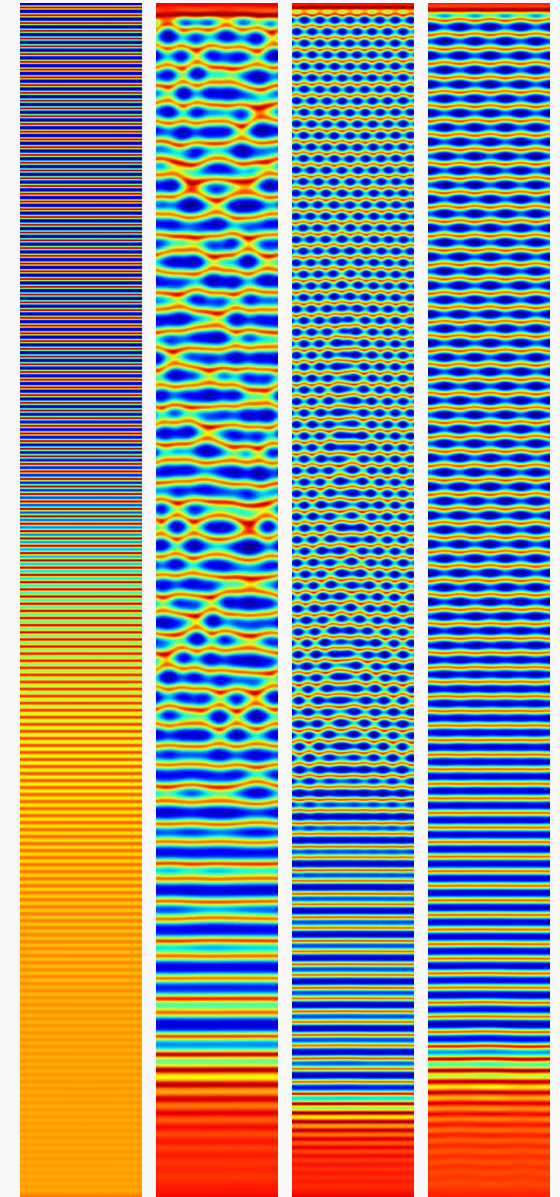
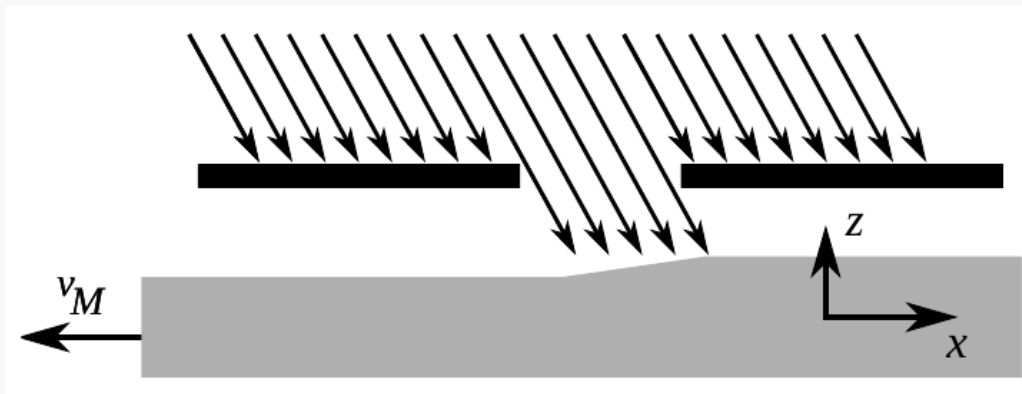
People communicate and spend, people make money , money attracts opinion...

Instability when there's too much money:



Different: surface-roughening and ion beams

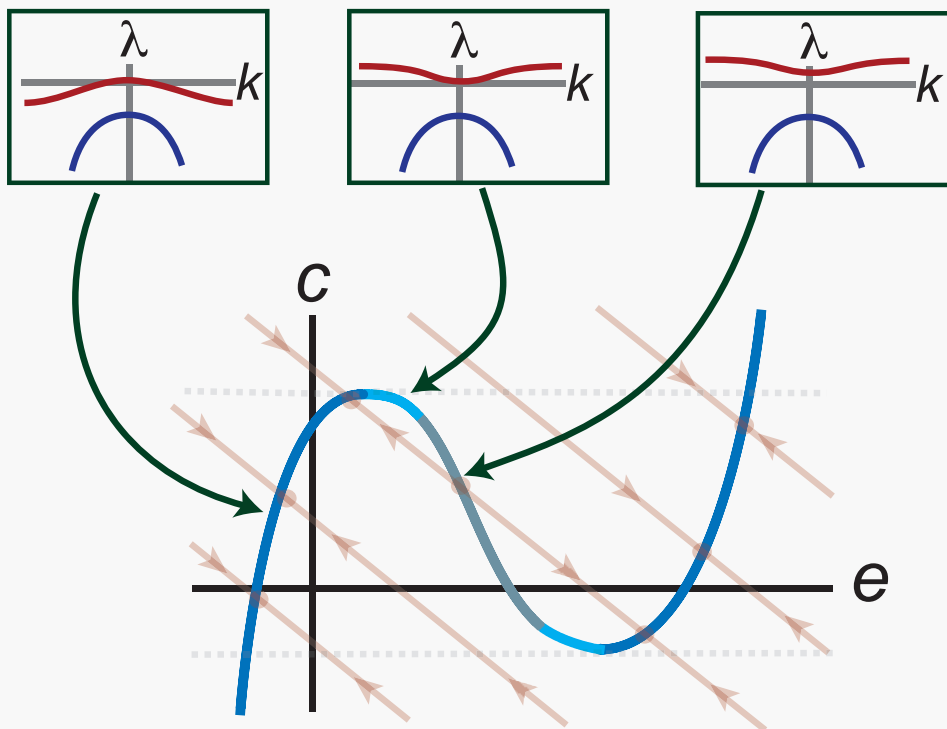
- Surface bombardement with ion beams → **instabilities**
 - surface roughness on nano-scales;
 - highly disordered structure
 - but masked fronts create **highly organized** surface ripples, nano-dots, ...
- [Gelfand&Bradley]



Pattern formation: fronts versus noise

$$\begin{cases} c_t = \Delta c - e(1-e)(e-a) - \gamma c \\ e_t = e(1-e)(e-a) + \gamma c \end{cases}$$

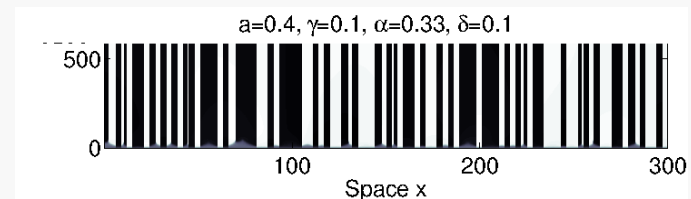
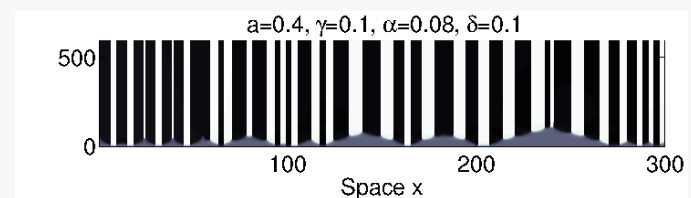
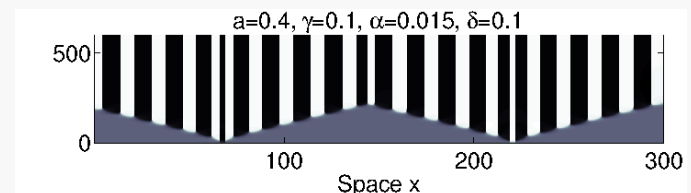
Linear Stability of equilibria



Perturbing $e = a, c = 0$
random amplitudes



random locations

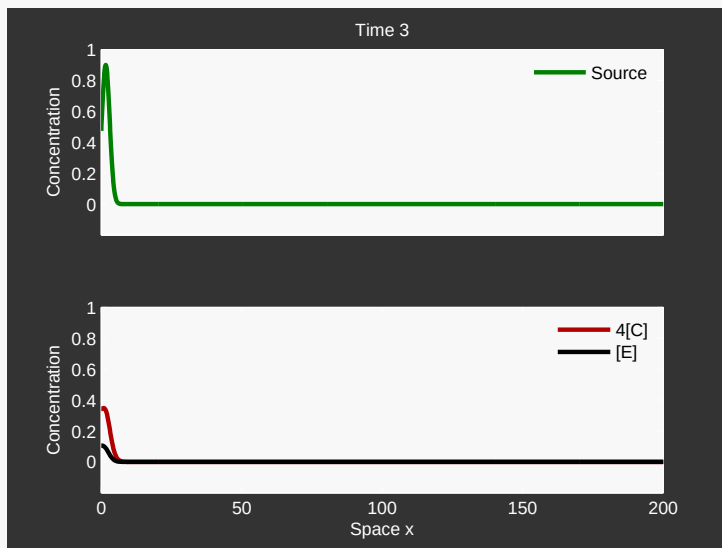


Invasion fronts: free and triggered

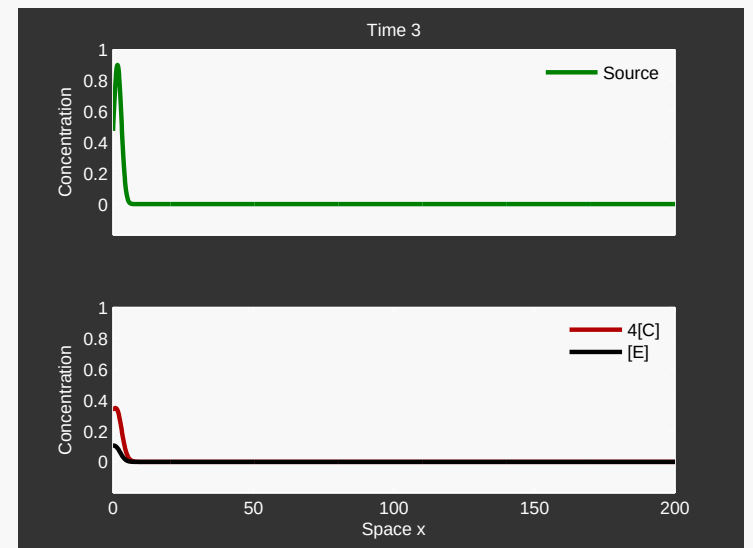
Spatio-temporal source term $h(t, x)$, depositing mass

$$\begin{cases} c_t = \Delta c - f(c, e) + h(t, x) \\ e_t = \kappa \Delta e + f(c, e) \end{cases}$$

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

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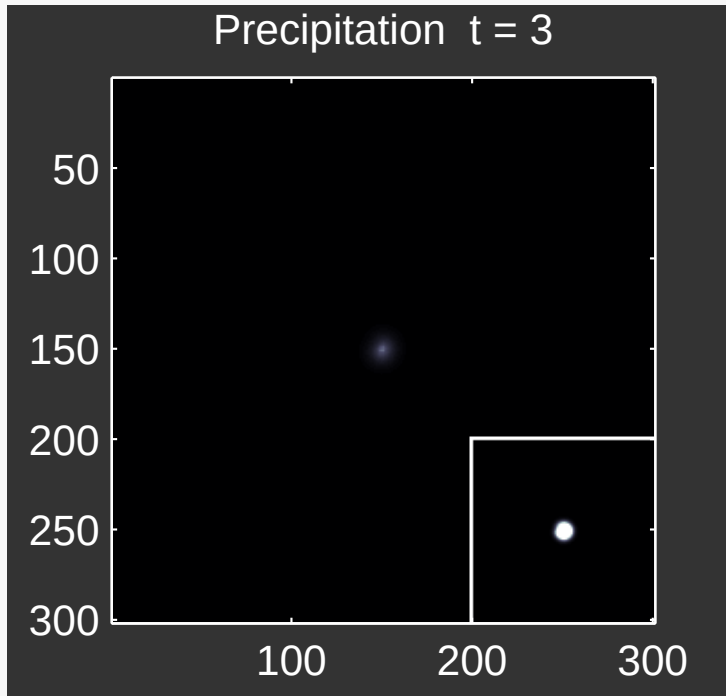
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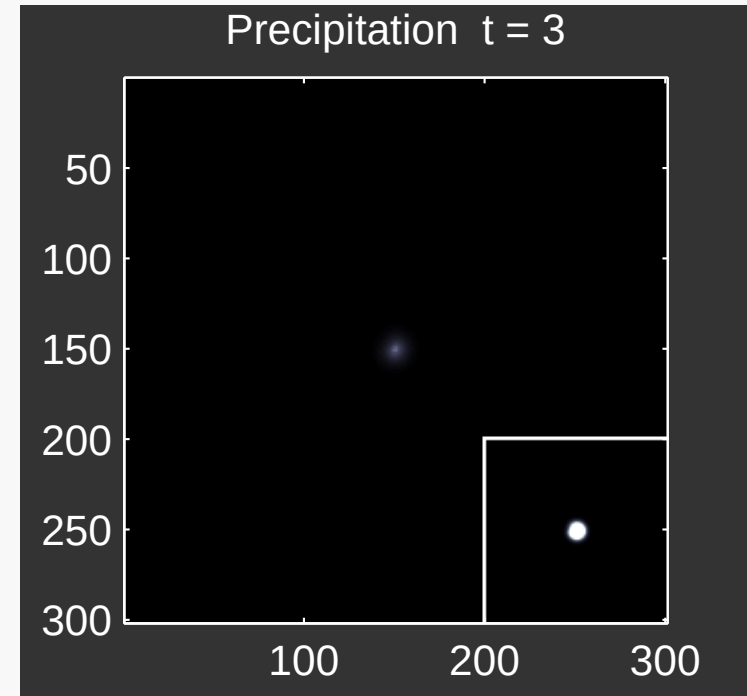
Slow source $s \ll 1$

Multi-dimensional patterns

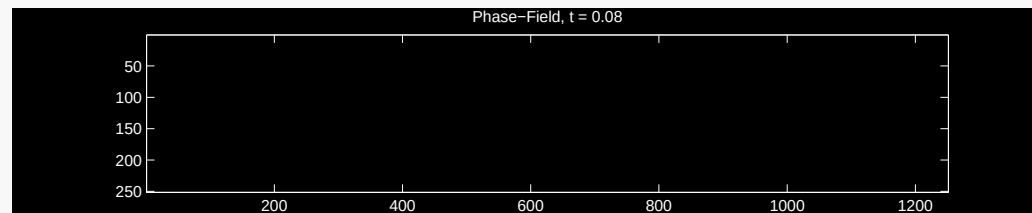
A plethora of patterns from “growth” and “threshold conversion”:



Wet stamping — isotropic



— anisotropic



trigger front and inhomogeneity

Multi-dimensional patterns

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Existence of invasion fronts

Two approaches:

Robustness:

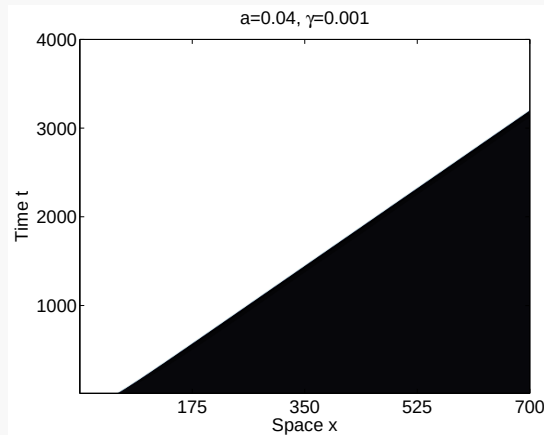
Show that linearization at a given front is Fredholm index 0 — without proving existence!

Existence:

Show that fronts exist using Conley's index!

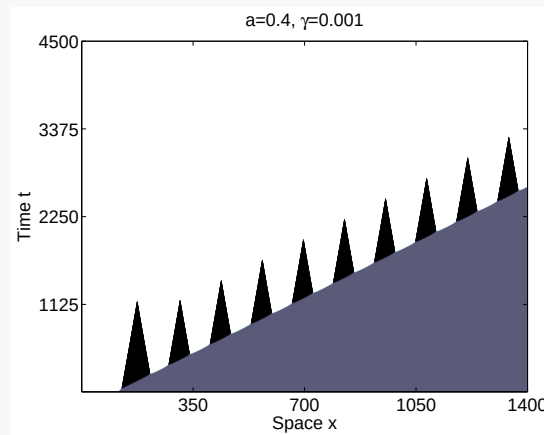
Robustness — phenomena

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



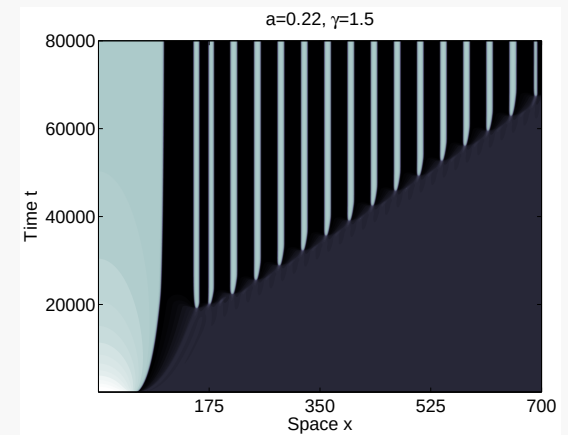
$\gamma = 0.001$, $a = 0.04$

Bulk Front



$\gamma = 0.001$, $a = 0.4$

Transient Pattern



$\gamma = 1.5$, $a = 0.22$

Persistent Pattern

$$c_t = c_{xx} - e(1 - e)(e - a) - \gamma c$$

$$e_t = de_{xx} + e(1 - e)(e - a) + \gamma c$$

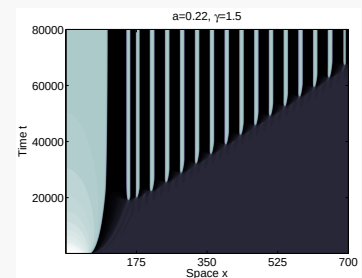
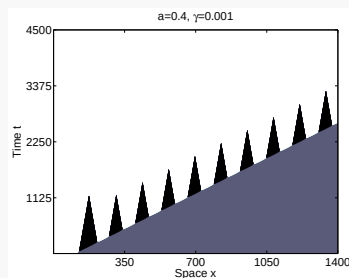
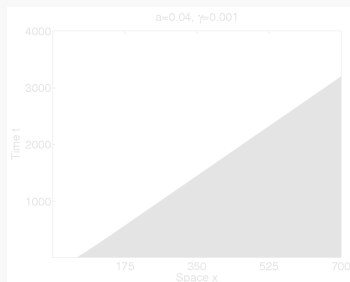
Robustness — results

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 $a_*(d) \dots$



Robustness — proofs

- Traveling-wave equation for $u = (c, e)(x - st, kx)$ as dyn' sys'

$$u_\xi = -k\partial_y u + v$$

$$v_\xi = -k\partial_y v - D^{-1} (F(u) + c(v - k\partial_y u))$$

Robustness — proofs

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

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- 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 $i_M(u_*^\pm)$? $\longrightarrow$ **Homotopies!**

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

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

Idea: Homotope $u_* = u_*^- \dots u_*^+$ and count ν 's crossing $i\mathbb{R}$

Resonant modes and Morse indices

How do we compute $i_M(u_*^\pm)$? $\longrightarrow$ **Homotopies!**

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

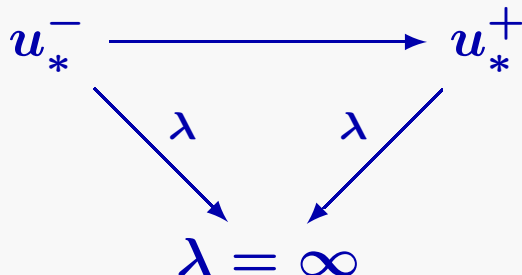
$$-s\nu u = D(k\partial_y + \nu)^2 u + F'(u_*)u$$

Idea: Homotope $u_* = u_*^- \dots u_*^+$ and count ν 's crossing $i\mathbb{R}$

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

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

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



Crossings in λ



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

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

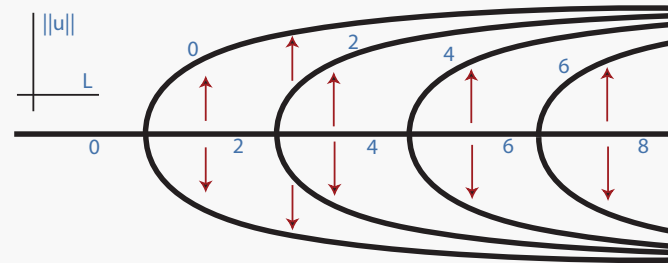
Gradient structure

$$u_t = -\nabla_{H^{-1}} E(u)$$

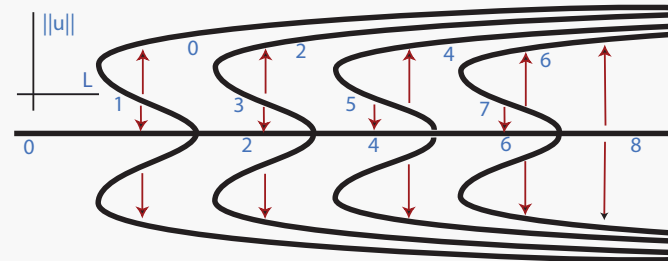
Equilibria and attractors

Dynamics on attractor: equilibria and heteroclinic connections

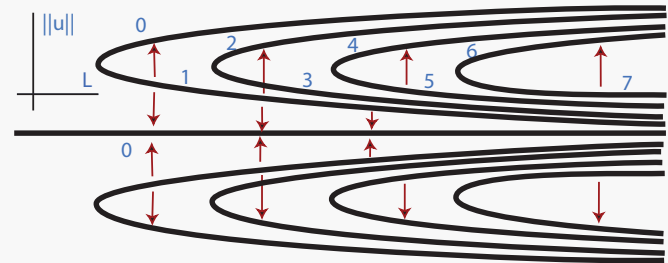
$$|m| < \frac{1}{\sqrt{5}}$$



$$\frac{1}{\sqrt{5}} < |m| < \frac{1}{\sqrt{3}}$$



$$\frac{1}{\sqrt{3}} < |m| < 1$$



[Grinfeld, Novick-Cohen]

Spinodal decomposition fronts

Main Theorem [S.]

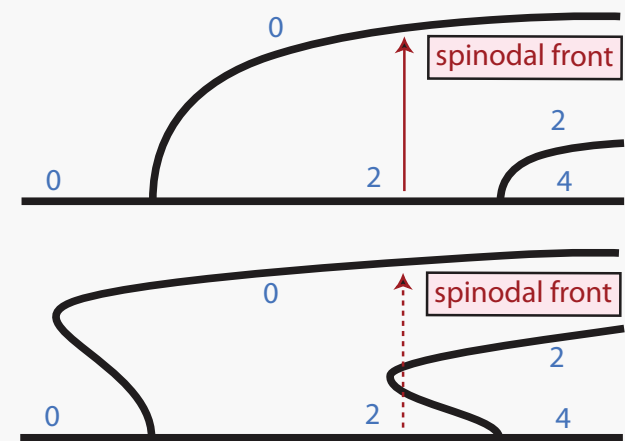
For each $|m| < 1/\sqrt{3}$, there exists a modulated front solution

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

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

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 $u_{*,1}, \dots, u_{*,j}$ so that the last wave connects to $u_{-,j}$ with minimal period $2\pi/k_{\text{lin}}$.



Existence — Outline

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

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

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

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

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

$$\int_\xi \int_\tau (\phi_{\xi\xi}^2 + \phi_\xi^4) \chi(\xi) < \infty, \quad \int_\xi \left(\oint_\tau su - \mathcal{I} \right)^2 < \infty$$

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- Galerkin approximations in τ , a priori estimates, give Conley index of bounded solutions as isolated invariant set
- Morse indices and connection matrices [Franzosa],[Mischaikow]

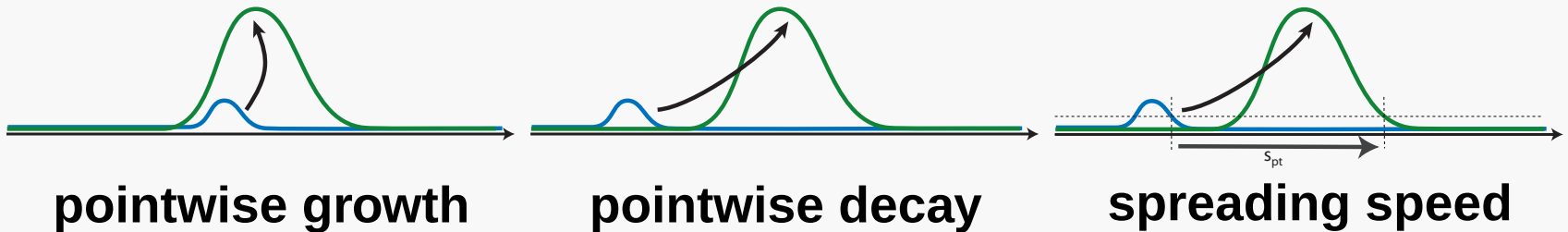
→ heteroclinic orbits

Outline

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

Spreading speeds

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



Linear dispersion relation

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

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

Pointwise growth modes (λ, ν) :

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

$$\partial_\nu D(\lambda, \nu) = 0 + \text{"pinching"}$$

Classic "Lemma": Typically,

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

Pointwise spreading speed:

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

Selected wavenumber:

$$k_{\text{lin}} = \omega_{\text{lin}} / s_{\text{pt}} \text{ where } i\omega_{\text{lin}} \text{ neutral pointwise growth mode at}$$

Spreading speeds — subtleties

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

- linear speeds $<$ “pinched speed”

$$u_t = u_x + u, \quad v_t = -v_x + v$$

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

- linear speed $<$ nonlinear speed: $\longrightarrow$ pushed fronts

$$u_t = u_{xx} + u(1 - u)(u - a), \quad a < 1/3$$

- nonlinear speed $<$ linear speed $\longrightarrow$ Lotka-Volterra
- linear speed $<$ nonlinear speed: $\longrightarrow$ staged invasion

Related question: What happens in the wake of invasion?

Spreading speeds — multi-d

Consider isotropic system, initial conditions $u_{\text{cpt}}(x)e^{iky}$.

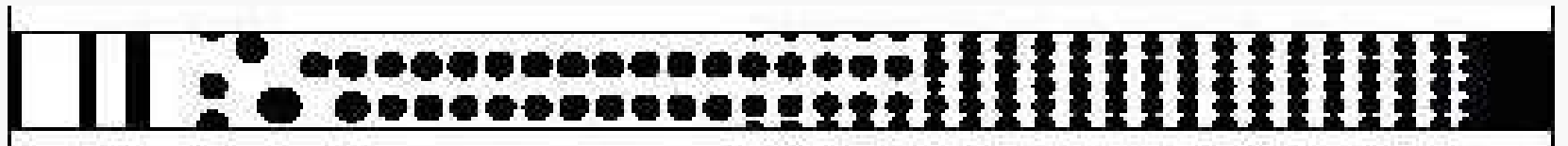
Define transverse modulated spreading speeds $s_{\text{lin}}(k)$

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

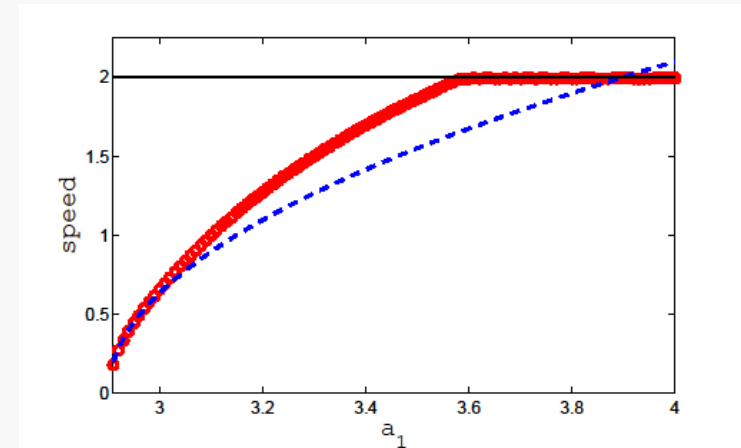
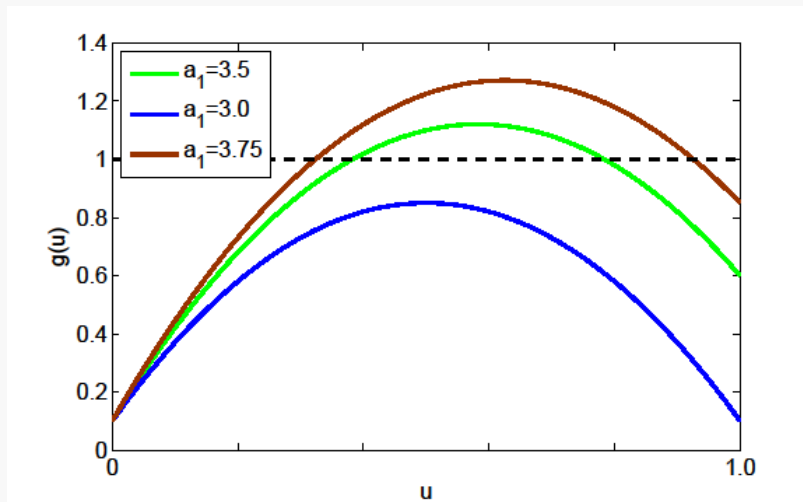
$$u_t = u_{xx} + u(1 - u)$$

$$v_t = dv_{xx} + g(u)v - v^3$$

“Instantaneous” v -speed:

$$s_v = -2\sqrt{dg(u)}$$

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

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

Resonance pole λ_{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:

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

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

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

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

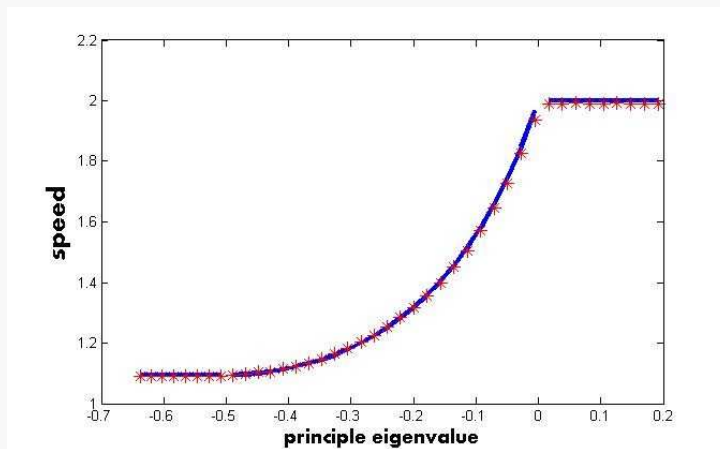
$$\frac{1}{2\nu_v^+} \log(\lambda_{rp}) \text{ if } 2\nu_v^+ - \nu_v^- > 0$$
$$\frac{1}{\nu_v^- \nu_v^+} \log(\lambda_{rp}) \text{ if } 2\nu_v^+ - \nu_v^- < 0$$

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

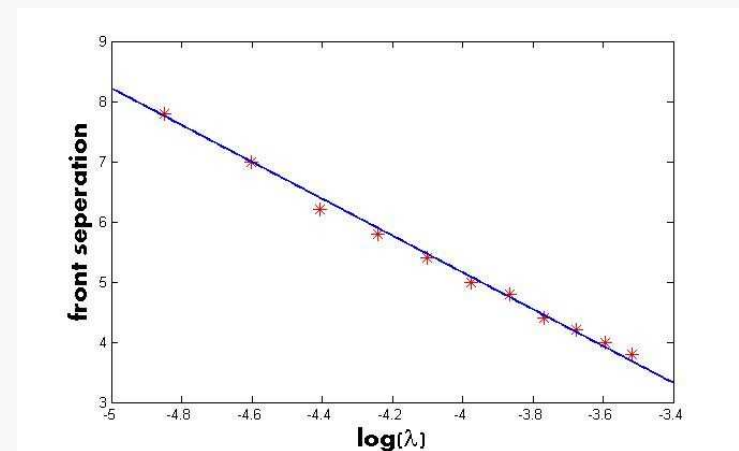
Comparison with simulations

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:

R Goh, S Mesuro, A Scheel, *Spatial wavenumber selection in recurrent precipitation*, SIADS 2011

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