The Stability and Dynamics of Localized Spot Patterns in the 2-D Gray-Scott Model

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Far-From Equilibrium Dynamics: January 2011

Kyoto Conference in Honor of Prof. Yasumasa Nishiura

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Outline of th Lecture

Overview: Localized Particle-Like Spot Solutions to RD systems in 2-D

1. **Brief History:** Self-Replicating Spots (Lab and Numerical Evidence)
2. **Phenomena and Terminology:** Competition Instabilities, Oscillatory Profile Instabilities, Spot Self-Replication Instabilities, Dynamically Triggered Instabilities.
3. Theoretical Approaches in 1-D and 2-D.

A Specific RD System in 2-D (Detailed Case Study)

1. **GS System:** Self-Replication, Oscillatory, and Competition Instabilities, of Spots in 2-D Planar Domains. Phase Diagrams for These Instabilities for Simple Spot Patterns. Ph.D work of Wan Chen (UBC, Postdoc Oxford).
2. **Some Open Issues:** A few interesting problems.

Singularly Perturbed RD Models: Localization

Spatially localized solutions can occur for singularly perturbed RD models

$$v_t = \varepsilon^2 \triangle v + g(u,v)\,; \quad \tau u_t = D \triangle u + f(u,v)\,, \quad \partial_n u = \partial_n v = 0\,, \quad x \in \partial\Omega\,.$$

Since $\varepsilon \ll 1$, v can be localized in space as a spot, i.e. concentration at a discrete set of points in $\Omega \in \mathbb{R}^2$.

Semi-Strong Interaction Regime: $D = O(1)$ so that u is global. We will focus on the this regime.

Weak Interaction Regime: $D = O(\varepsilon^2)$ so that u is also localized. Pioneering studies of Nishiura and Ueyama (1999,2001) are for this regime.

Some Simple Kinetics: (There is No Variational Structure)

- **GS Model:** (Pearson, 1993; scaling of Muratov-Osipov)

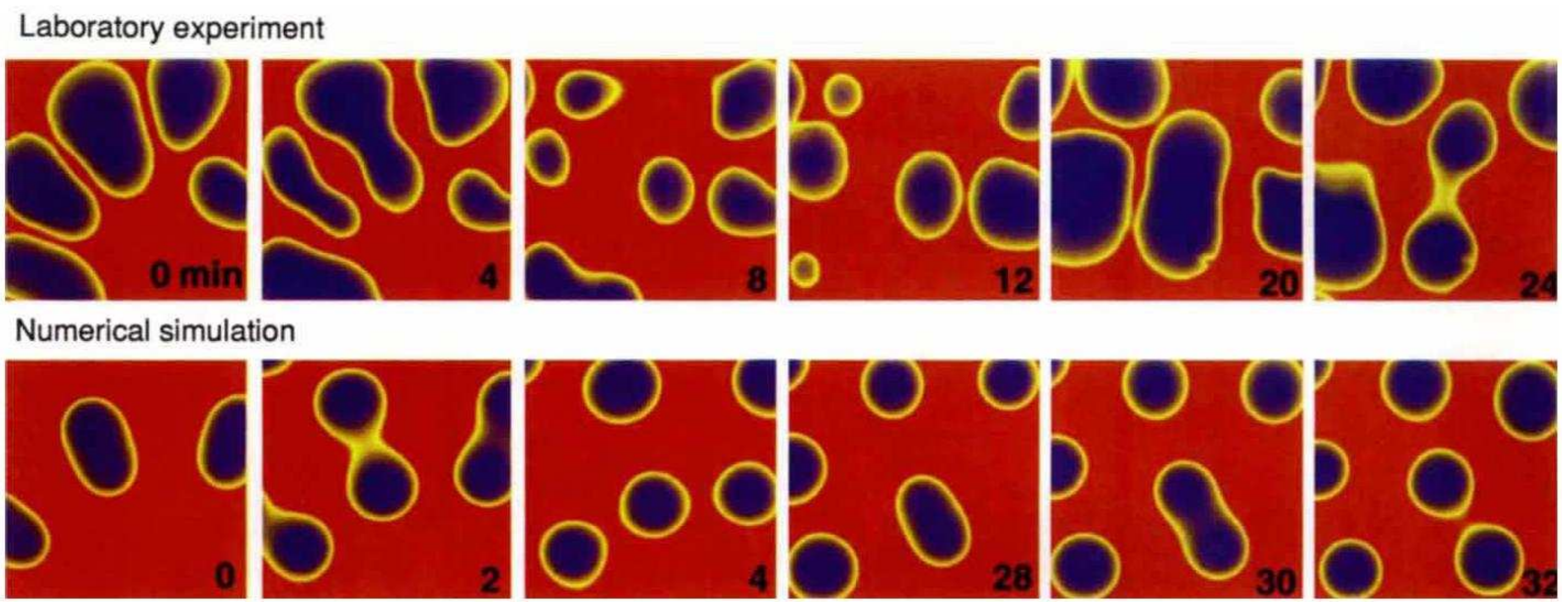
$$g(u,v) = -v + Auv^2\,, \qquad f(u,v) = (1-u) - uv^2\,.$$

- **Schnakenburg Model:** $g(u,v) = -v + uv^2$ and $f(u,v) = a - uv^2$.
- **GM Model:** $g(u,v) = -v + v^2/u$ and $f(u,v) = -u + v^2$.

Self-Replicating Spots: Overview I

Experimental evidence of spot-splitting

- The Ferrocyanide-iodate-sulphite reaction. (Swinney et al., Nature, V. 369, (1994), pp. 215-218). The numerical simulations are for GS model by Pearson (Science, 1993).

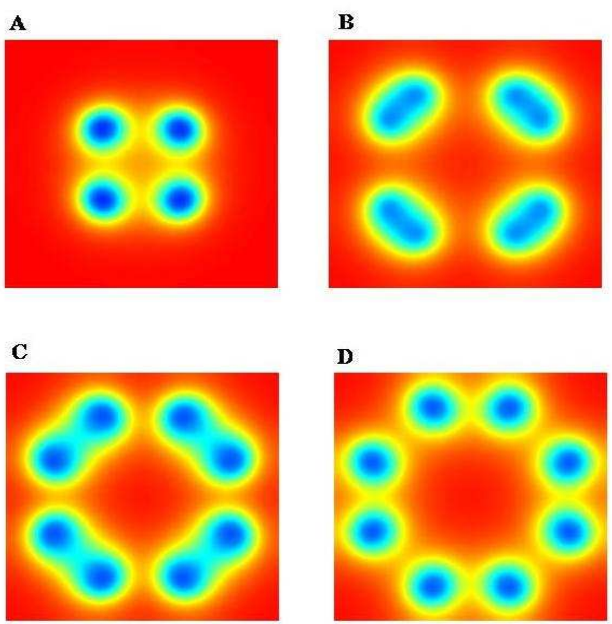


- A planar gas discharge system. (Astrov & Purwins, Phys. Lett. A, V. 283, (2001), pp. 349-354. Such systems often modeled by 3-component RD systems.

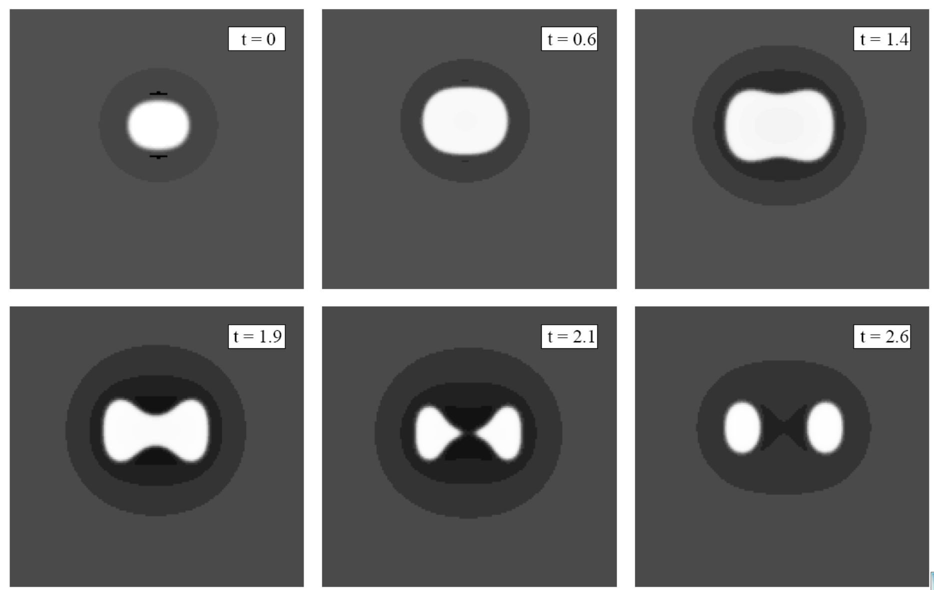
Self-Replicating Spots: Overview II

Numerical evidence of spot-splitting

- Pearson, *Complex Patterns in a Simple System*, Science, **216**.
- Nishiura & Ueyama, *Spatial-Temporal Chaos in the Gray-Scott model*, Physica D, **150**, (2001), p. 137; *Skeleton Structure of Self-Replicating Dynamics*, Physica D, **130**, (1999), p. 73.
- Muratov & Osipov, *Scenarios of Domain Pattern Formation in Reaction-Diffusion Systems*, Phys. Rev. E, **54**, (1996), pp. 4860–4879.



Left: Pearson (1993).



Right: Muratov and Osipov (1996).

Self-Replicating Spots: Overview III

(More Recent) Numerical evidence of spot-splitting

- **Schnakenburg Model:**
  - J. Zhu et al., *Application of Discontinuous Galerkin Methods for RD Systems in Developmental Biology*, J. Sci. Comput., (2010)
  - A. Madvamuse, P. Maini, *Velocity-Induced Numerical Solutions of RD Systems on Continuously Growing Domains*, JCP, **225**, (2007), p. 100.
  - **Growing Domains:** numerics showing spot-splitting for the Schnakenburg model on a slowly growing planar domain (Madvamuse, Maini, 2006)
- Golovin, Matkowsky, Volpert, *Turing Patterns for the Brusselator with Superdiffusion*, SIAP, **68**, (2008), p. 251.
- K. Glasner, *Spatially Localized Structures in Diblock Copolymer Mixtures*, SIAP, (2010). (Self-replication of worm-like patterns in 2-D).

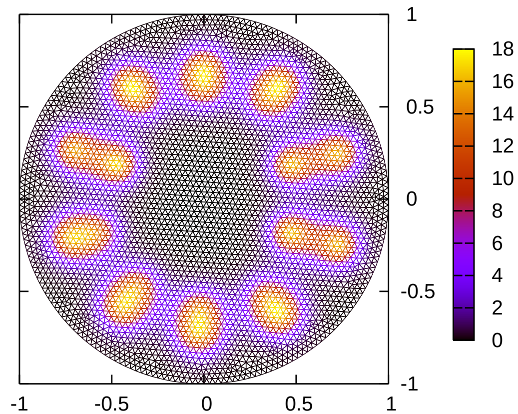
Self-Replicating Spots: Overview IV

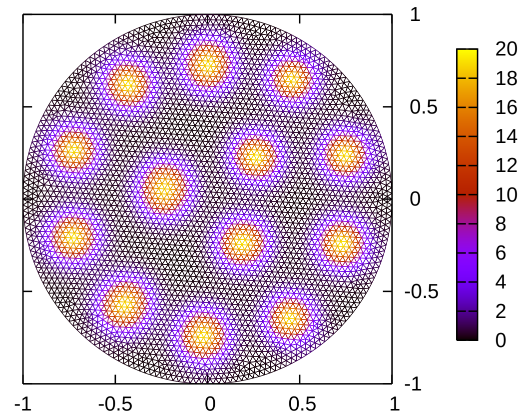
Spot patterns arise from generic initial conditions, or from the breakup of a stripe to varicose instabilities: Spot-replication appears here as a secondary instability.

2-D GS Model: Semi-Strong Regime.

$$v_t = \varepsilon^2 \triangle v - v + A u v^2 \,, \quad \tau u_t = D \triangle u - (1-u) - u v^2 \,.$$

Parameters: $A = 3.87$, $D = 1$, $\varepsilon = 0.04$, $\tau = 1$: (Movie)





Ref: KWW, *Zigzag and Breakup Instabilities of Stripes and Rings....* Stud. Appl. Math., **116**, (2006), pp. 35–95.

Three Types of Instabilities

Dynamically triggered instability is an instability triggered at some later time by the slow dynamics of a collection of spots as they evolve towards their equilibrium locations. Bifurcations induced by intrinsic motion, not by externally varying control parameter.

Competition Instability: (Movie)

Oscillatory Instability: (Movie)

Self-Replication Instability: (Movie 1) (Movie 2) (Movie 3)

Questions: Predict instability types, determine dynamics etc...

Theoretical Approaches

- **1) Turing Stability Analysis:** linearize RD around a spatially homogeneous steady state. Look for diffusion-driven Turing instabilities.
- **2) Weakly Nonlinear Theory:** capture nonlinear terms in multi-scale perturbative way and derive normal form amplitude equations.
  - With regards to the intricate patterns computed by him for the GS model (Science 1993), Pearson (Los Alamos) remarks: *Most work in this field has focused on pattern formation from a spatially uniform state that is near the transition from linear stability to linear instability. With this restriction, standard bifurcation-theoretic tools such as amplitude equations have been used with considerable success (ref: Cross and Hohenburg (Rev. Mod. Physics 1993)). It is unclear whether the patterns presented here will yield to these standard technologies.*
- **3) Stability of Localized Pulse-Type Structures:** Study the existence, stability, and dynamics of localized spike (1-D) and spot patterns (2-D).
  - Different approaches in 1-D: geometric singular perturbation theory Lyapunov-Schmidt, NLEP analysis, matched asymptotics, renormalization group theory. What about 2-D?

Theoretical Approaches: Brief History I

- **Brief History of 1-D Theory: Spike Solutions to RD System**
  - Early formal 1-D studies of self-replication of spikes for GS; Petrov, Scott, Schowalter (1994), Reynolds, Ponce-Dawson, et al. (1998).
  - Pulse-splitting “qualitative” mechanism for the GS model in the weak interaction regime $D = O(\varepsilon^2)$ based on global bifurcation scenario (Nishiura, Ei, Ueyama, (1999–)).
  - Dynamics and stability of exponentially weakly interacting pulses (Ei, Nishiura, Sandstede...)
  - Stability and dynamics of pulses for the GM and GS models in the semi-strong regime (Doelman, Gardner, Kaper, Promislow, Muratov, Osipov, Iron, MJW, Kolokolnikov, Chen, Wei) dating from 1997–. Notable here is the NLEP stability analysis of pulses, the SLEP method for spikes, and the study of self-replication of pulses for GS model in 1-D.
  - Rigorous framework in 1-D for 2-spike dynamics for GM model in semi-strong regime based on renormalization group methods (Doelman, Kaper, Promislow, 2007).

Theoretical Approaches: Brief History II

Brief History of 2-D Theory: Spot Solutions to RD Systems

- Repulsive interactions of spots in weak interaction regime (Ei, Mimura, Ohta...)
- Scattors etc..; Strong Interactions; Phase III Nishiura et al.
- NLEP stability theory of equilibrium spot patterns for GM and GS in semi-strong interaction regime (Wei-Winter, (2001–)). NLEP problems arise from leading-order terms in infinite logarithmic expansion in ε. Lyapunov-Schmidt analyses for existence of equilibrium spots.
- One-Spot dynamics for GM (X. Chen, Kowalczyk, Kolokolnikov, MJW, (2001–)).

Remarks:

- For spot patterns in arbitrary 2-D domains, a PDE-based approach based on Green's functions is needed, as the ODE-based tools of geometric singular perturbation theory for 1-D are of more limited use.
- **Largely Open:** Give an analytical theory for self-replication of spots, dynamics of spots, and other instabilities (oscillatory and competition) in arbitrary 2-D planar domains. Focus on semi-strong regime.

GS Model: Detailed Case Study

GS Model: in a 2-D domain Ω consider the GS model

$$v_t = \varepsilon^2 \Delta v - v + A u v^2 \,, \quad \partial_n v = 0 \,, \quad x \in \partial\Omega$$

$$\tau u_t = D \Delta u + (1 - u) - u v^2 \,, \quad \partial_n u = 0 \,, \quad x \in \partial\Omega \,.$$

- Consider semi-strong limit $\varepsilon \to 0$ with $D = O(1)$.
- There are three key parameters $D > 0$, $\tau > 0$, $A > 0$.
- Three main instabilities: self-replication (large A), oscillatory instability (large τ), competition or overcrowding instability (large D).
- Obtain a phase diagram classification for various “symmetric” arrangements of spots. Determine parameter ranges for dynamically triggered instabilities.
- W. Chen, M. J. Ward, *The Stability and Dynamics of Localized Spot Patterns in the Two-Dimensional Gray-Scott Model*, revision under review SIAM J. Appl. Dyn. Sys. (2010), (69 pages).
- T. Kolokolnikov, M.J. Ward, J. Wei, *Spot Self-Replication and Dynamics for the Schnakenburg Model...* J. Nonl. Sci., 19, (2009), pp. 1–56.

Our Theoretical Framework: 2-D Spot Patterns

- **Quasi-Equilibrium Pattern:** Use singular perturbation methodology to construct quasi-steady pattern consisting of localized spots in arbitrary 2-D planar domains. Key issue: derive a quasi-equilibrium pattern that is accurate to all orders in $-1/\log \varepsilon$, i.e. "sum the log expansion".
- **Dynamics:** Derive dynamics of spots in terms of collective coordinates characterizing the pattern. The dynamics is slow wrt ϵ.
- **Stability:** For $O(1)$ time-scale instabilities, derive and study singularly perturbed eigenvalue problems in semi-strong interaction regime.
  1. **Self-replication** instability is largely a local instability near a spot.
  2. **Competition and Oscillatory** instabilities are studied through certain globally coupled eigenvalue problems. To leading-order in $-1/\log \varepsilon$, the global eigenvalue problem reduces to the scalar Nonlocal Eigenvalue Problems (NLEP's) of Wei-Winter (2001–).

Remarks: This approach is widely applicable and

- Various Green's functions play a central role.
- "Similar" to studying vortex dynamics (GL model of superconductivity).
- **Difficulty:** Need a more rigorous understanding.

GS Model: Quasi-Equilibrium I

Key: Matched asymptotic expansion approach tailored to problems with logarithmic gauge functions.

For spots located at x_j for $j = 1, .., K$, in the j^{th} inner region we define y, U_j, V_j, by

$$y = \varepsilon^{-1}(x - x_j)\,, \quad \rho = |y|\,, \quad u = \frac{\varepsilon}{A\sqrt{D}} U_j\,, \quad v = \frac{\sqrt{D}}{\epsilon} V_j\,.$$

The spots are found to drift slowly with speed $\mathcal{O}(\varepsilon^2)$, and so we “freeze” their locations in the asymptotic construction of the quasi equilibrium.

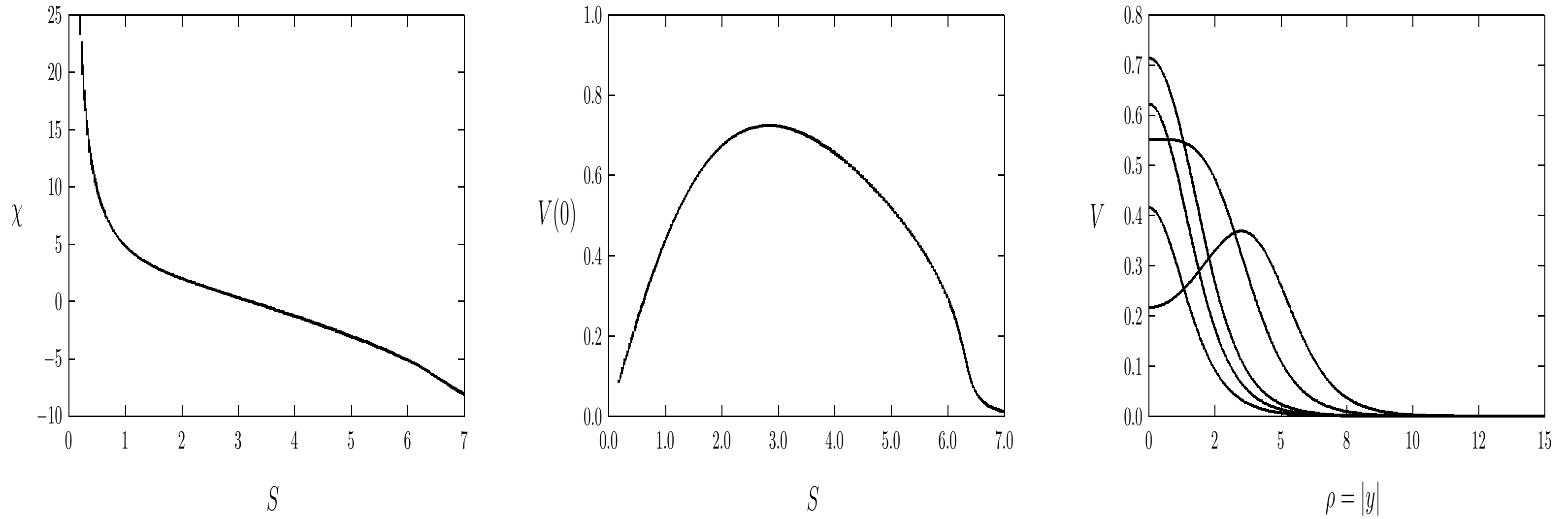
To within $\mathcal{O}(\varepsilon)$ terms, U_j and V_j satisfy the radially symmetric core problem on $\rho \geq 0$:

$$V_{j\rho\rho} + \frac{1}{\rho} V_{j\rho} - V_j + U_j V_j^2 = 0\,, \qquad U_{j\rho\rho} + \frac{1}{\rho} U_{j\rho} - U_j V_j^2 = 0\,,$$

$$V_j \to 0\,, \qquad U_j \sim S_j \log \rho + \chi(S_j) + o(1)\,, \quad \text{as} \quad \rho \to \infty\,.$$

Here $S_j = \int_0^\infty \rho U_j V_j^2 \, d\rho > 0$ is termed the “source strength” (to be found by matching to an outer solution). Solutions to the core problem and the nonlinear function $\chi(S_j)$ are obtained numerically.

GS Model: Quasi-Equilibrium II



Left: $\chi(S_j)$; **Middle:** $V_j(0)$ vs. S_j; **Right:** $V_j(\rho)$ for a few S_j.

- Numerically; there is a unique solution to core problem on $0 < S_j < 7$.
- $V_j(\rho)$ has a volcano shape when $S_j > S_v \approx 4.78$.
- The function $\chi(S_j)$ is central to constructing quasi-equilibria.
- Thus, the "ground-state problem" is a coupled set of BVP in contrast to the scalar BVP $w_{\rho\rho} + \rho^{-1} w_\rho - w + w^2 = 0$ of NLEP theory.
- For $S_j \ll 1$, V_j is well-approximated by the scalar ground-state w.
- **Difficulty:** No rigorous existence theory for solutions to the coupled core problem.

GS Model: Quasi-Equilibrium III

- In the outer region $v \ll 1$, each spot is a "source" for u in that

$$uv^2 \sim \frac{2\pi\epsilon\sqrt{D}}{A}\sum_{j=1}^{K}\left(\int_0^\infty \rho U_j V_j^2\, d\rho\right)\,\delta(x-x_j) \sim \frac{2\pi\epsilon\sqrt{D}}{A}\sum_{j=1}^{K} S_j\delta(x-x_j)\,.$$

- The matching condition is that the local and global representations of u must agree as $x \to x_j$ and $|y| \to \infty$.

In this way, the outer or global u satisfies

$$D\Delta u + (1-u) = \frac{2\pi\sqrt{D}\,\varepsilon}{A}\sum_{j=1}^{K} S_j\,\delta(x-x_j)\,, \quad \text{in } \Omega\,; \quad \partial_n u = 0\,, \quad \text{on } \partial\Omega\,,$$

$$u \sim \frac{\varepsilon}{A\sqrt{D}}\Big(S_j \ln|x-x_j| - S_j \ln\varepsilon + \chi(S_j)\Big)\,, \quad \text{as } x \to x_j\,, \quad j = 1, \ldots, K\,.$$

Matching has provided K singularity structures where the strength of each singularity and the regular part of each singularity is prescribed.

GS Model: Quasi-Equilibrium IV

This problem indicates that we should define ν and $\mathcal{A}$ by

$$\nu = -1/\ln\varepsilon\,, \qquad \mathcal{A} = \nu A\sqrt{D}/\varepsilon\,.$$

Then, the global u satisfies

$$\Delta u + \frac{(1-u)}{D} = \frac{2\pi\nu}{\mathcal{A}}\sum_{j=1}^{K} S_j\,\delta(x-x_j)\,, \quad \text{in } \Omega\,; \quad \partial_n u = 0\,, \quad \text{on } \partial\Omega\,,$$

$$u \sim \frac{1}{\mathcal{A}}\left(S_j\nu\ln|x-x_j| + S_j + \nu\chi(S_j)\right)\,, \quad \text{as } x\to x_j\,, \quad j=1,\ldots,K\,.$$

Key Point: A nonlinear algebraic system for S_j will be obtained since the form of the regular (or non-singular) part as $x\to x_j$ is pre-specified. More specifically, in solving

$$\Delta u - u = 2\pi\sum_{j=1}^{k} A_j\delta(x-x_j) \quad \text{in } \Omega\,; \qquad \partial_n u = 0 \quad \text{on } \partial\Omega\,,$$

$$u \sim A_i\ln|x-x_i| + B_i\,, \quad \text{as} \quad x\to x_i\,, \quad i=1,\ldots,K\,,$$

there is a relationship between the A_i and B_i for a solution to exist.

GS Model: Quasi-Equilibrium V

We represent u as

$$u = 1 - \frac{2\pi\nu}{\mathcal{A}} \sum_{j=1}^{K} S_j G(x; x_j)\,,$$

where $G(x; x_j)$ is the reduced-wave G-function with regular part R_{jj}:

$$\Delta G - \frac{1}{D} G = -\delta(x - x_j)\,, \quad \text{in } \Omega\,; \quad \partial_n G = 0\,, \quad x \in \partial\Omega\,,$$

$$G(x; x_j) \sim -\frac{1}{2\pi} \log|x - x_j| + R_{jj} + o(1)\,, \quad \text{as } x \to x_j\,.$$

From the regular part of the singularity structures, we obtain that the S_j for $j = 1, \ldots, k$ satisfy the nonlinear algebraic system:

$$\mathcal{A} = S_j + 2\pi\nu \left(S_j R_{j,j} + \sum_{\substack{i=1 \\ i \neq j}}^{K} S_i G_{j,i} \right) + \nu \chi(S_j)\,, \quad j = 1, \ldots, K\,,$$

$$\nu = -1/\ln\varepsilon\,, \qquad \mathcal{A} = \nu A \sqrt{D}/\varepsilon = A\sqrt{D}/\varepsilon(-\ln\varepsilon)\,.$$

Upon determining the S_j, we know the core solution near each spot.

GS Model: Quasi-Equilibrium VI

- For G and its regular part R, simple formulae for a disk and a rectangle (Ewald summation needed). Fast-multipole methods can be used for arbitrary Ω (Greengard et al.).
- Construction yields a quasi-equilibrium solution for any “frozen” configuration x_j, $j = 1, \ldots, K$ of spots. The error is smaller than any power of $\nu = -1/\log \varepsilon$; i.e. we have “summed” all logarithmic terms.
- **Related log expansion problems:** eigenvalue of the Laplacian in a domain with localized traps (Ozawa 1982–), Bratu’s equation with cooling rod, etc.. The novelty here with the GS model is that the inner problem is nonlinear. Typically, for Laplacian eigenvalue problems in a 2-D domain with small hole Ω_ε, the inner core problem is

$$\Delta_y U = 0\,, \quad y \notin \Omega_1 = \varepsilon^{-1}\Omega_\varepsilon\,; \quad U = 0\,, \quad y \in \partial\Omega_1\,,$$
$$U \sim \log|y| - \log d + o(1)\,, \quad |y| \to \infty\,,$$

  where d is the logarithmic capacitance. Our inner nonlinear core problem for one spot yields $U \sim S \log|y| + \chi(S) + o(1)$ as $|y| \to \infty$.
- **Survey** of strong localized perturbation theory: Online notes for Fourth Winter School Applied Math (City U. Hong Kong, Dec. 2010).

GS Model: Dynamics of Spots I

Key Point: The collective slow coordinates for the dynamics are S_j and x_j, for $j = 1, \ldots k$.

Principal Result: (DAE System): *Let $\mathcal{A} = \varepsilon A/(\nu\sqrt{D})$ and $\nu = -1/\log\varepsilon$. Provided that there are no $\mathcal{O}(1)$ time-scale instabilities of the quasi-equilibrium profile, the DAE system for the time evolution of the source strengths S_j and spot locations x_j is*

$$\mathcal{A} = S_j + 2\pi\nu\left(S_j R_{j,j} + \sum_{\substack{i=1\\ i\neq j}}^{K} S_i G_{j,i}\right) + \nu\chi(S_j)\,, \quad j = 1, \ldots, K$$

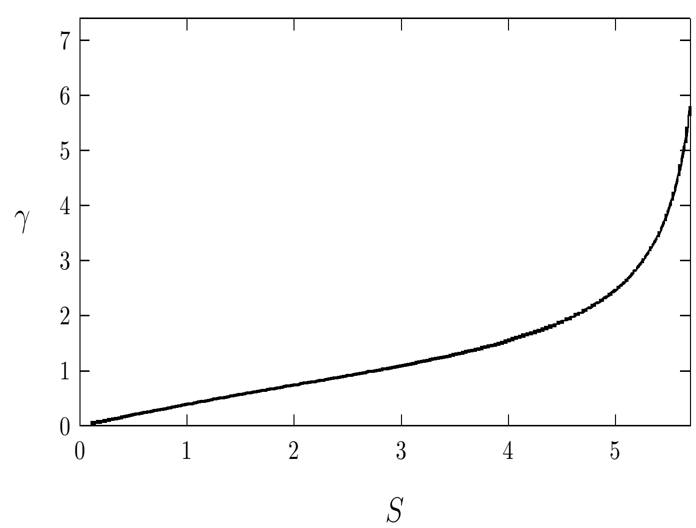
$$x_j' \sim -2\pi\varepsilon^2\gamma(S_j)\left(S_j \nabla R(x_j; x_j) + \sum_{\substack{i=1\\ i\neq j}}^{K} S_i \nabla G(x_j; x_i)\right)\,, \quad j = 1, \ldots, K\,.$$

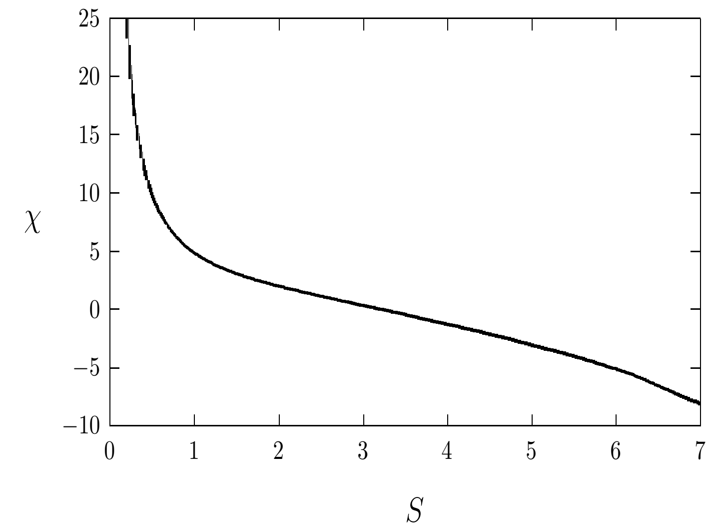
Here $G_{j,i} \equiv G(x_j; x_i)$ and $R_{j,j} \equiv R(x_j; x_j)$, where $G(x; x_j)$ is the Reduced Wave Green's function with regular part $R(x_j; x_j)$, which depend on D.

Note: The speed of the spots is $\mathcal{O}(\varepsilon^2)$.

GS Model: Dynamics of Spots: II

- The DAE system depends on two functions $\gamma(S_j)$ and $\chi(S_j)$ associated with the coupled core problem near each spot.





Left: γ vs. S_j **Right:** χ vs. S_j

- The Green's function terms G_{ij} and R_{jj}, which mediate spot interactions, depend on D and the shape of Ω.
- **Universality:** Changing the nonlinearities, while maintaing that the "outer" solution is $D\Delta u - u = \sum_j \beta_j \delta(x - x_j)$ will change only $\gamma(S_j)$ and $\chi(S_j)$.

GS Model: Dynamics of Spots: III

Sketch of Derivation: In the inner region, we expand to higher order

$$u = \frac{\varepsilon}{A\sqrt{D}} \left(U_{0j}(\rho) + \varepsilon U_{1j}(\mathbf{y}) + \ldots \right) , \qquad v = \frac{\sqrt{D}}{\varepsilon} \left(V_{0j}(\rho) + \varepsilon V_{1j}(\mathbf{y}) + \ldots \right) .$$

where $y = \varepsilon^{-1}(x - x_j)$ with $x_j = x_j(\varepsilon^2 t)$.

Define $w_j \equiv (V_{1j}, U_{1j})^T$. The GS model yields

$$\Delta_{\mathbf{y}} w_j + \mathcal{M}_j w_j = g_j \, , \qquad y \in \mathbb{R}^2 \, ,$$

where

$$\mathcal{M}_j \equiv \begin{pmatrix} -1 + 2U_0 V_0 & V_0^2 \\ -2U_0 V_0 & -V_0^2 \end{pmatrix} , \quad g_j \equiv \begin{pmatrix} -V_0' x_j' \cdot y / |y| \\ 0 \end{pmatrix} .$$

The matching condition for the algebraic in ε terms is:

$$w_j \to \begin{pmatrix} 0 \\ -f_j \cdot y \end{pmatrix} \text{ as } \quad y \to \infty \, ; \quad f_j \equiv 2\pi \left(S_j \nabla R(\mathbf{x}_j; \mathbf{x}_j) + \sum_{i \neq j}^{K} S_i \nabla G(\mathbf{x}_j; \mathbf{x}_i) \right)$$

GS Model: Dynamics of Spots: IV

Lemma: *A necessary condition for the existence of a solution for* w_j *is that*

$$x_j' = \gamma(S_j) f_j \,, \qquad \gamma \equiv \gamma(S_j) = \frac{-2}{\int_0^\infty \rho V_0'(\rho) \hat{\Phi}^*(\rho)\, d\rho} \,.$$

Here $\hat{\Phi}^*(\rho)$ *is the first component of the radially symmetric adjoint solution* $\hat{P}^*(\rho) \equiv \left(\hat{\Phi}^*(\rho), \hat{\Psi}^*(\rho)\right)^t$ *satisfying*

$$\partial_{\rho\rho}\hat{P}^* + \rho^{-1}\partial_\rho \hat{P}^* - \rho^{-2}\hat{P}^* + \mathcal{M}_0^t \hat{P}^* = \mathbf{0} \,, \quad 0 < \rho < \infty \,,$$

subject to $\hat{\Phi}^* \to 0$ *exponentially and* $\hat{\Psi}^* \sim 1/\rho$ *as* $\rho \to \infty$.

Derivation: standard solvability condition type argument.

GS Model: The Stability of Quasi-Equilibria

We seek fast $\mathcal{O}(1)$ time-scale instabilities relative to slow dynamics of x_j.

We assume $\tau \ll \mathcal{O}(\varepsilon^{-2})$. Let $u = u_e + \mathrm{e}^{\lambda t}\eta$ and $v = v_e + \mathrm{e}^{\lambda t}\phi$. In each **inner region** we introduce the local angular mode $m = 0, 2, 3, \ldots$ by

$$\eta = \frac{\varepsilon}{A\sqrt{D}} e^{im\theta} N_j(\rho)\,, \quad \phi = \frac{\sqrt{D}}{\varepsilon} e^{im\theta} \Phi_j(\rho)\,, \quad \rho = |y|\,, \quad y = \varepsilon^{-1}(x - x_j)\,.$$

Then, on $0 < \rho < \infty$, we get the two-component eigenvalue problem

$$\mathcal{L}_m \Phi_j - \Phi_j + 2U_j V_j \Phi_j + V_j^2 N_j = \lambda \Phi_j\,, \quad \mathcal{L}_m N_j - 2U_j V_j \Phi_j - V_j^2 N_j = 0\,,$$

with operator $\mathcal{L}_m$ defined by

$$\mathcal{L}_m \Phi_j \equiv \partial_{\rho\rho} \Phi_j + \rho^{-1} \partial_\rho \Phi_j - m^2 \rho^{-2} \Phi_j\,.$$

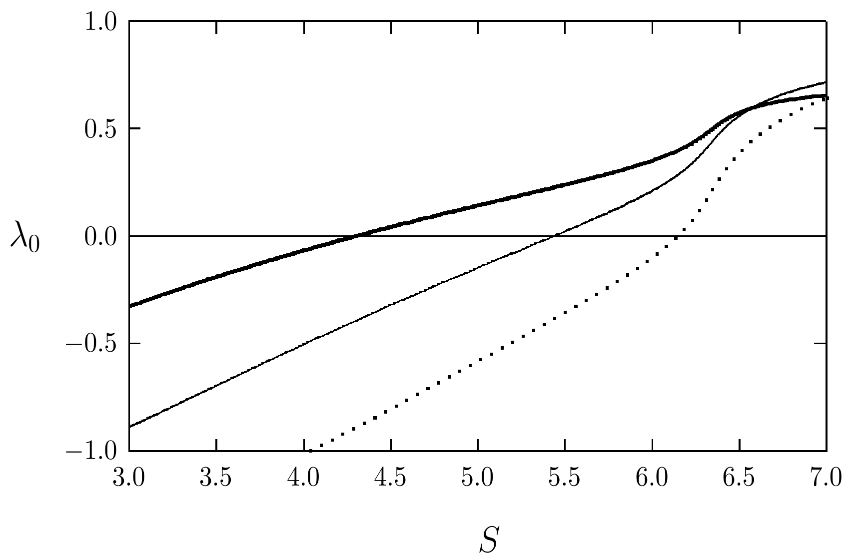
- U_j and V_j are computed from the core problem and depend on S_j. The S_j for $j = 1, \ldots, K$ satisfy the nonlinear algebraic system involving G.
- **Key Point:** This is a two-component eigenvalue problem, in contrast to the scalar problem of NLEP theory. Hence, with no maximum principle there is no ordering principle for eigenvalues wrt number of nodal lines of eigenfunctions.

GS Model: Self-Replication Instability I

Definition of Thresholds: Let $\lambda_0(S_j, m)$ denote the eigenvalue with the largest real part, with Σ_m denoting the S_j s.t. Re$\lambda_0(\Sigma_m, m) = 0$.

The Modes $m \geq 2$: We must impose $N_j \sim \rho^{-2} \to 0$ as $\rho \to \infty$. Thus, the local eigenvalue problems are uncoupled, except through the determination of S_j. We compute

$$\Sigma_2 = 4.303\,, \quad \Sigma_3 = 5.439\,, \quad \Sigma_4 = 6.143\,.$$



Key point: The peanut-splitting instability $m = 2$ is dominant.

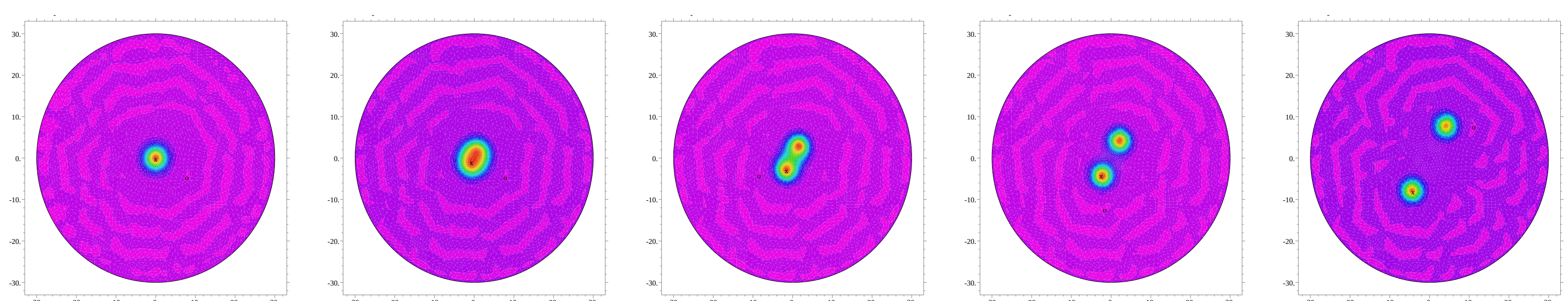
GS Model: Self-Replication Instability II

Principal Result: *Consider the GS model with $\varepsilon \ll 1$, $\tau \ll \mathcal{O}(\varepsilon^{-2})$, $\mathcal{A} = \varepsilon A/(\nu\sqrt{D})$ so that $A = \mathcal{O}(-\varepsilon \ln \varepsilon)$. Then, if $S_j < \Sigma_2 \approx 4.31$, the j^{th} spot is linearly stable to a spot deformation instability for modes $m \geq 2$. Alternatively, for $S_j > \Sigma_2$, it is linearly unstable to the peanut-splitting mode $m = 2$.*

Numerically: This instability triggers a nonlinear self-replication event for the time-dependent elliptic-parabolic nonlinear core problem

$$V_t = \Delta_y V - V + UV^2 \,, \qquad \Delta_y U - UV^2 = 0 \,, \quad y \in \mathbb{R}^2 \,,$$

$$V \to 0 \,, \quad U \to S \ln |y| \,, \quad \text{as } |y| \to \infty \,.$$

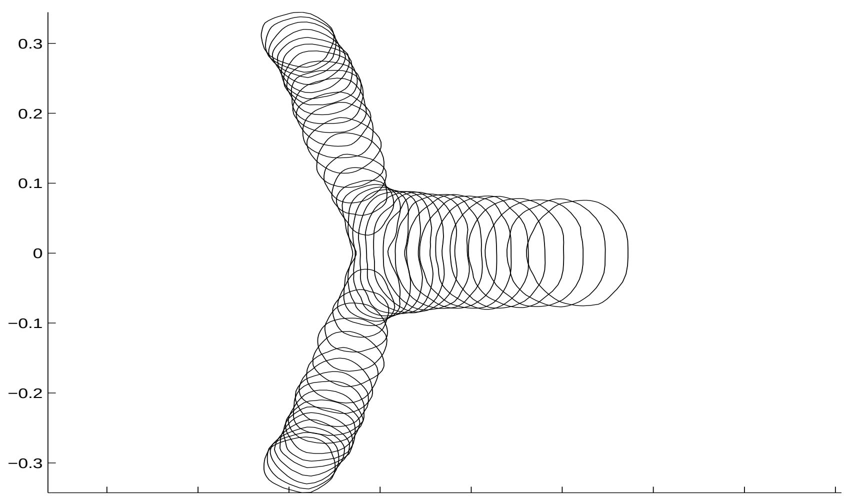


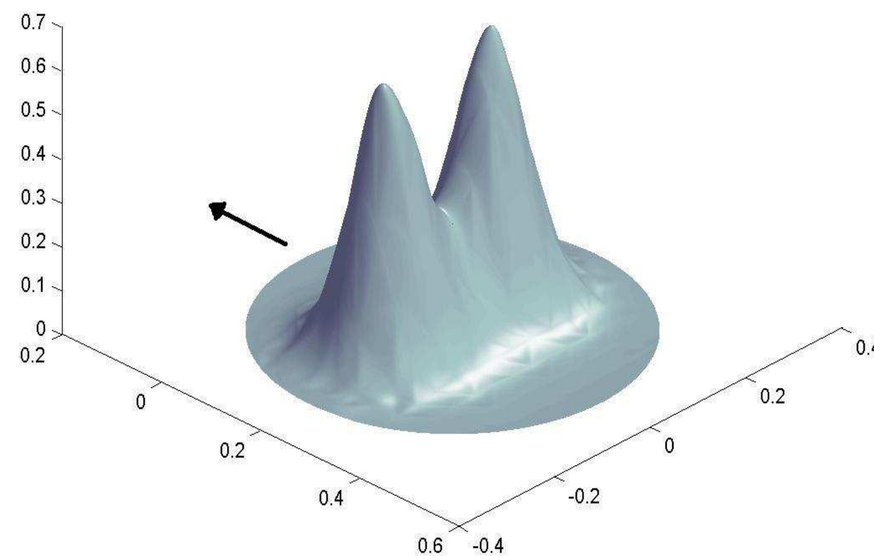
Plots at $t = 0, 100, 130, 140, 170$ for disk of radius 30 when $S = 4.5$.

GS Model: Self-Replication Instability III

- For $S_j \approx \Sigma_2$, the linearization of the core problem has an approximate four-dimensional null-space (two translation and splitting modes).
- By a projection onto this four-dimensional nullspace (center manifold-type reduction), it can be shown that splitting occurs in a direction perpendicular to the motion when $\varepsilon \ll 1$. **Ref:** Kolokolnikov, MJW, Wei, J. Nonlin. Sci. (2009).

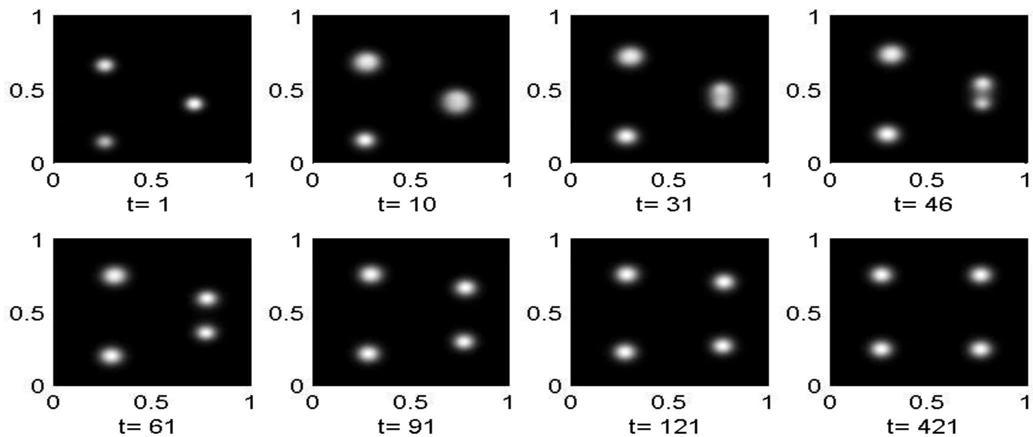
Spot-Splitting in the Unit Disk: $x_0(0) = (0.5, 0.0)$, $\varepsilon = 0.03$, Left: Trace of the contour $v = 0.5$ from $t = 15$ to $t = 175$ with increments $\Delta t = 5$. Right: spatial profile of v at $t = 105$ during the splitting.
(Movie for unit square with $S = 5.0 > \Sigma_2$)



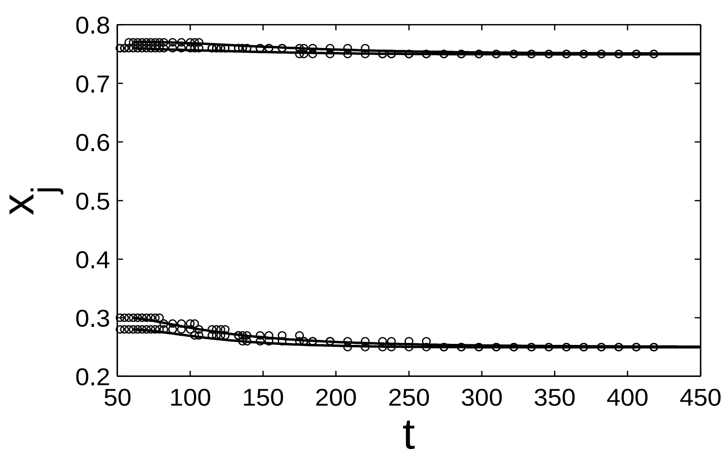


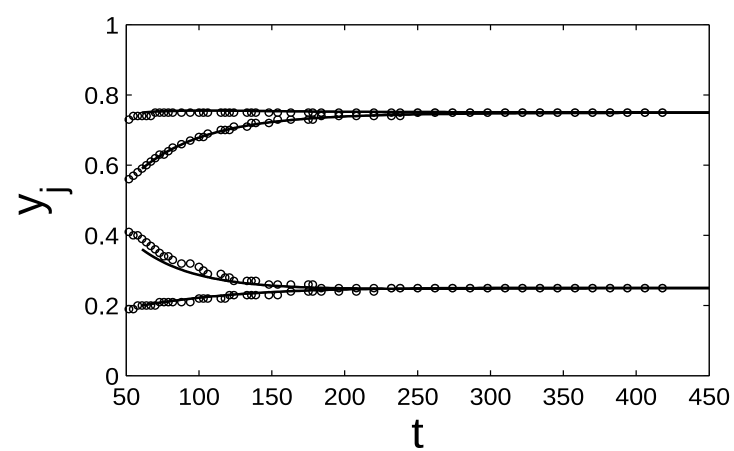
GS Model: Self-Replication Instability IV

Example: Fix $\mathcal{A} = 20$, $D = 1$, $\varepsilon = 0.02$. Put $K = 3$ spots on a ring of radius $r = 0.3$ centered at $(0.4, 0.4)$ in the unit square at $t = 0$. We compute $S_1 = 4.05$, $S_2 = 2.37$, $S_3 = 4.79$. Predict: One spot splits beginning at $t = 0$ (Movie)



DAE Dynamics accurately tracks spots after splitting event





Competition and Oscillatory Instabilities I

Key Point: These are instabilities associated with locally radially symmetric perturbations near a spot, i.e. $m = 0$.

When $m = 0$, the local eigenvalue problem for $N_j = N_j(\rho)$ and $\Phi_j = \Phi_j(\rho)$, with $\rho = |\mathbf{y}|$, near the j^{th} spot is

$$\Phi_j'' + \frac{1}{\rho}\Phi_j' - \Phi_j + 2U_jV_j\Phi_j + V_j^2 N_j = \lambda\Phi_j\,, \quad \rho \geq 0\,; \quad \Phi_j'(0) = 0\,,$$

$$N_j'' + \frac{1}{\rho}N_j' - V_j^2 N_j - 2U_jV_j\Phi_j = 0\,, \quad \rho \geq 0\,; \quad N_j'(0) = 0\,,$$

$$\Phi_j(\rho) \to 0\,, \quad N_j(\rho) \to C_j \ln\rho + C_j\hat{B}_j + o(1)\,, \quad \text{as} \quad \rho \to \infty.$$

- For $\rho \gg 1$ the operator for N_j reduces to $N_j'' + \rho^{-1}N_j' \approx 0$ for $\rho \gg 1$, and so we cannot impose that $N_j \to 0$ as $\rho \to \infty$. Instead, we must allow for logarithmic growth at infinity, which allows us to match to the outer solution.
- The constant $\hat{B}_j$ is a function of λ and S_j.

Competition and Oscillatory Instabilities II

In the outer region each spot is a "source" for the outer eigenfunction η. Recall that $\eta = \varepsilon/(A\sqrt{D})N_j(\rho)$. Matching condition: LHS and RHS agree as $x \to x_j$ and $\rho \to \infty$.

In this way, the outer eigenfunction with $\partial_n \eta = 0$ on $\partial\Omega$ satisfies

$$\Delta\eta - \frac{(1+\tau\lambda)}{D}\eta = \frac{2\pi\varepsilon}{A\sqrt{D}} \sum_{j=1}^{k} C_j \delta(x - x_j)\,, \quad \text{in } \ x \in \Omega$$

$$\eta \sim \frac{\varepsilon}{A\sqrt{D}} \left[C_j \ln|x - x_j| + \frac{C_j}{\nu} + C_j \hat{B}_j + o(1) \right]\,, \quad \text{as } \ x \to x_j\,, \ \ j = 1, \ldots, K\,.$$

Key: We have K singularity structures where both the singular and regular parts are specified. We write η as

$$\eta = -\frac{2\pi\varepsilon}{A\sqrt{D}} \sum_{j=1}^{K} C_j G_\lambda(x; x_j)\,,$$

where the λ-dependent Green's function satisfies

Competition and Oscillatory Instabilities III

$$\Delta G_\lambda - \frac{(1+\tau\lambda)}{D} G_\lambda = -\delta(x - x_j)\,, \quad x \in \Omega\,; \qquad \partial_n G_\lambda = 0\,, \quad x \in \partial\Omega\,,$$

$$G_\lambda(x; x_j) \sim -\frac{1}{2\pi} \ln|x - x_j| + R_{\lambda\, j,j} + o(1) \quad \text{as} \quad x \to x_j\,.$$

Note: $R_{\lambda j,j}$ depends on x_j, D, and $\tau\lambda$. The regular parts of the singularity structures yield a homogeneous linear system for C_j:

$$C_j\,(1 + 2\pi\nu R_{\lambda\, j,j}) + \nu C_j \hat{B}_j + 2\pi\nu \sum_{i\neq j}^{K} C_i G_{\lambda\, i,j} = 0\,, \quad j = 1, \ldots, K\,.$$

By writing as a matrix problem $\mathcal{M}c = 0$, then $\det(M) = 0$ determines λ.

- **Global Coupling is in Two Ways:** Recall that S_j are also coupled globally (and that $\hat{B}_j = \hat{B}_j(S_j, \lambda)$). Formulation is an extended-NLEP problem accounting for all logarithmic correction terms ν.
- Certainly similar to the asymptotic approach for determining the eigenvalue of the Laplacian in 2-D in a domain with K small holes (Keller, MJW, (1993)).

Competition and Oscillatory Instabilities IV

In matrix form, the globally coupled extended-NLEP problem is

$$\mathcal{M}\,\mathbf{c} = \mathbf{0}\,, \qquad \mathcal{M} \equiv I + \nu\mathcal{B} + 2\pi\nu\mathcal{G}_\lambda\,,$$

where $\mathbf{c} \equiv (C_1, \ldots, C_k)^T$, and the matrices $\mathcal{G}_\lambda$ and $\mathcal{B}$ are

$$\mathcal{G}_{\lambda j,j} = R_{\lambda jj}\,, \quad \mathcal{G}_{\lambda i,j} = \mathcal{G}_{\lambda j,i} = G_\lambda(x_i; x_j)\,, \;\; i \neq j\,; \quad \mathcal{B} = \text{Diag}(\hat{B}_j)$$

Note: $\mathcal{G}_\lambda$ is symmetric matrix, but is not Hermitian when λ is complex.

Also, the nonlinear algebraic system for the S_j can be written as:

$$\mathcal{A}\mathbf{e} = \mathbf{s} + 2\pi\nu\mathcal{G}_0\mathbf{s} + \nu\mathcal{X}\,,$$

where $\mathbf{e} = (1, \ldots, 1)^t$, $\mathbf{s} = (S_1, \ldots, S_k)^T$, and $\mathcal{X} = \text{Diag}(\chi(S_j))$.

Principal Result: *For $A = \mathcal{O}(-\varepsilon\ln\varepsilon)$, and $\tau\lambda \ll \mathcal{O}(\varepsilon^{-2})$, the stability of a K-spot pattern to locally radially symmetric perturbations near each spot is determined by det$(\mathcal{M}) = 0$. If the principal eigenvalue λ_0 satisfies Re$(\lambda_0) < 0$, then the $K-$spot quasi-equilibrium solution is linearly stable to such perturbations near each spot, otherwise it is linearly unstable.*

Competition and Oscillatory Instabilities V

- **Oscillatory:** For $k \geq 1$, as τ is increased a c.c eigenvalue pair can cross into Re$(\lambda_0) > 0$ (Hopf bifurcation). In certain cases, one can predict $\mathbf{c} = (1, \ldots, 1)^T$ (i.e. a synchronous oscillatory instability). **Numerically: it initiates an oscillatory death in the amplitude of spots. Subcritical?**
  - **Note:** There is no such instability generated by the core problem alone; i.e. imposing N_j bounded at infinity, then no Hopf bifurcation occurs. Oscillation results from the global coupling.
- **Competition:** For $k \geq 2$, as D is increased, a real eigenvalue λ_0 can enter unstable right half-plane along the real axis Im$(\lambda_0) = 0$. In certain cases, one can predict $\mathbf{c} = (1, -1, 1, -1, ...)^T$ (i.e. a sign fluctuating instability). **Numerically: it initiates a spot competition process leading to annihilation of some spots.**
- **Hybrid Asymptotic-Numerical Formulation:** If $\mathcal{G}_\lambda$ is analytically available, only simple numerics is needed: solving BVP's, root-finders, etc.
- **Key Feature in 2-D:** The three instabilities occur in the same parameter regime $\mathcal{A} = \mathcal{O}(1)$, $D = \mathcal{O}(1)$ when we do not make the leading-order $\nu \ll 1$ approximation. Thus, compute phase diagrams for instabilities. Not true for GS in 1-D.

Competition and Oscillatory Instabilities VI

Phase Diagrams: for "Symmetric" spot configurations. Assume that $\mathbf{x}_1, \ldots, \mathbf{x}_k$ is such that $\mathcal{G}_\lambda$ is a circulant matrix.

This occurs for two-spots in $\mathbb{R}^2$; for K spots equally spaced on a ring concentric with unit disk; for two spots in a arbitrary Ω when $R_{\lambda 1,1} = R_{\lambda 2,2}$ holds, etc...("equivalent" to equally-spaced spike patterns in $\mathbb{R}^1$).

Lemma: *For the $k \times k$ symmetric and circulant Green's matrix $\mathcal{G}_\lambda$ whose first row vector is $\mathbf{a} = (a_1, \ldots, a_k)$, the spectrum $\mathcal{G}_\lambda v = \omega_\lambda v$ is*

$$\begin{cases} \omega_{\lambda 1} & = \sum_{m=1}^{k} a_m, \quad v_1^T = (1, \ldots, 1), \\ \omega_{\lambda j} & = \sum_{m=0}^{k-1} \cos\left(\frac{2\pi(j-1)\,m}{k}\right) a_{m+1}, \quad \text{multiplicity 2}, \\ \mathbf{v}_j^T & = \left(1, \cos\left(\frac{2\pi(j-1)}{k}\right), \ldots, \cos\left(\frac{2\pi(j-1)(k-1)}{k}\right)\right), \\ \mathbf{v}_{k+2-j}^T & = \left(0, \sin\left(\frac{2\pi(j-1)}{k}\right), \ldots, \sin\left(\frac{2\pi(j-1)(k-1)}{k}\right)\right), \quad j = 2, \ldots, \lceil k/2 \rceil + 1\,. \end{cases}$$

Note: $\lceil m \rceil$ is smallest integer not less than m. Note: If k is even, then a simple eigenvector is $(1, -1, \cdots, 1, -1)^T$.

Competition and Oscillatory Instabilities VII

Simplifications Owing to Circulant Matrix Condition

- **(Quasi-Equilibria)** There are solutions with a common source strength S_c, where S_c satisfies

$$\mathcal{A} = S_c + 2\pi\nu\theta S_c + \nu\chi(S_c)\,,$$

where $\mathcal{G}_0\mathbf{e} = \theta\mathbf{e}$, $\mathbf{e} = (1,\ldots,1)^T$.

- **(Extended-NLEP Problem)** The global eigenvalues are the roots of K transcendental equations for λ:

$$f_j \equiv 1 + \nu\hat{B}_c + 2\pi\nu\omega_{\lambda j}(\tau\lambda) = 0\,,$$

where $\omega_{\lambda j}(\tau\lambda)$ for $j = 1,\ldots,K$ is any eigenvalue of $\mathcal{G}_\lambda$, and $\mathbf{c}_j = \mathbf{v}_j$. Note that $\hat{B}_c = \hat{B}_c(S,\lambda)$ is independent of j (need one core problem

- **(Threshold for $\lambda = 0$)** obtained by solving the coupled problem

$$1 + \nu\chi'(S_c) + 2\pi\nu\omega_{0j}(0) = 0\,, \quad \mathcal{A} = S_c + 2\pi\nu\theta S_c + \nu\chi(S_c)\,,$$

where $\omega_{0j}(0)$ is any of the eigenvalues of $\mathcal{G}_0$. **Key:** $\hat{B}_c(0,S_c) = \chi'(S_c)$.

Two-Spot Pattern in $\mathbb{R}^2$: I

Put two spots at $x_1 = (-\alpha, 0)$ and $x_2 = (\alpha, 0)$. Set $D = 1$ and $\varepsilon = 0.02$.

With $S_1 = S_2 \equiv S_c$, the common source strength S_c satisfies

$$A = \frac{\varepsilon}{\nu}\mathcal{F}(S_c)\,; \qquad \mathcal{F}(S_c) \equiv S_c\left[1 + \nu(\ln 2 - \gamma_e) + \nu K_0\left(2\alpha\right)\right] + \nu\,\chi(S_c)\,.$$

The existence and splitting thresholds are simply

$$A_{\text{exist}} = \frac{\varepsilon}{\nu}\min_{S_c}\left(\mathcal{F}(S_c)\right)\;; \quad A_{\text{split}} = \frac{\varepsilon}{\nu}\mathcal{F}(\Sigma_2)\,, \quad \Sigma_2 = 4.31\ldots\,.$$

(Repulsive) slow DAE dynamics for α: $d\alpha/d\xi = -\gamma(S_c)S_c K_0'\left(2\alpha\right) > 0$ and $A = \varepsilon\nu^{-1}\mathcal{F}(S_c)$.

Extended-NLEP Problem: The eigenpair $v_\pm$, $\omega_{\lambda\,j}(\tau\lambda)$ of $\mathcal{G}_\lambda$ are

$$\omega_{\lambda\,\pm} = \frac{1}{2\pi}\left[(\ln 2 - \gamma_e - \log\sqrt{1+\tau\lambda}) \pm K_0(2\alpha\sqrt{1+\tau\lambda})\right]\,, \quad \mathbf{v}_\pm \equiv (1, \pm 1)^T\,.$$

With $\hat{B}_c = \hat{B}_c(\lambda, S_c)$, we must determine the roots of

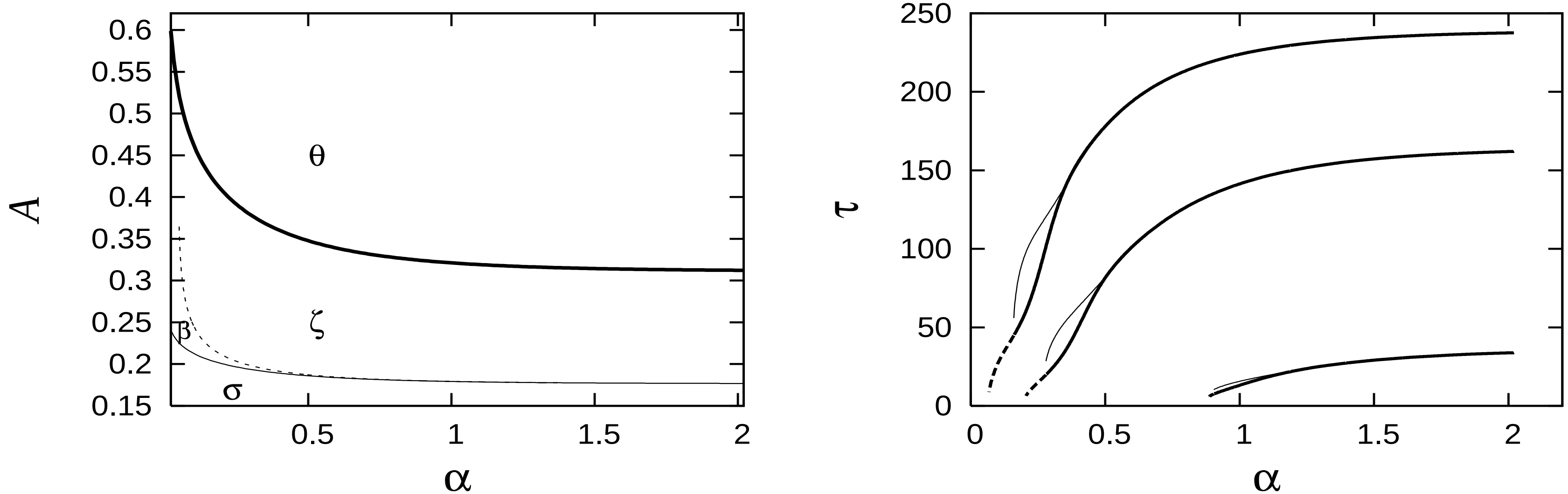
$$\nu^{-1} + \hat{B}_c + 2\pi\omega_{\lambda\,\pm}(\tau\lambda) = 0\,.$$

Two-Spot Pattern in $\mathbb{R}^2$: II

Competition Instability is set by v_-. To compute threshold $A = A_{\text{comp}}(\alpha)$, set $\lambda = 0$, $\hat{B}_c(0, S_c) = \chi'(S_c)$, and eliminate S_c between

$$\chi'(S_c) + \ln 2 - \gamma_e - K_0(2\alpha) = -\nu^{-1}\,, \qquad A = \frac{\varepsilon}{\nu}\mathcal{F}(S_c)\,.$$

Oscillatory Instability: We compute $\tau_+(\alpha)$ and $\tau_-(\alpha)$, and obtain $\tau_+ < \tau_-$ (synchronous oscillatory instability).

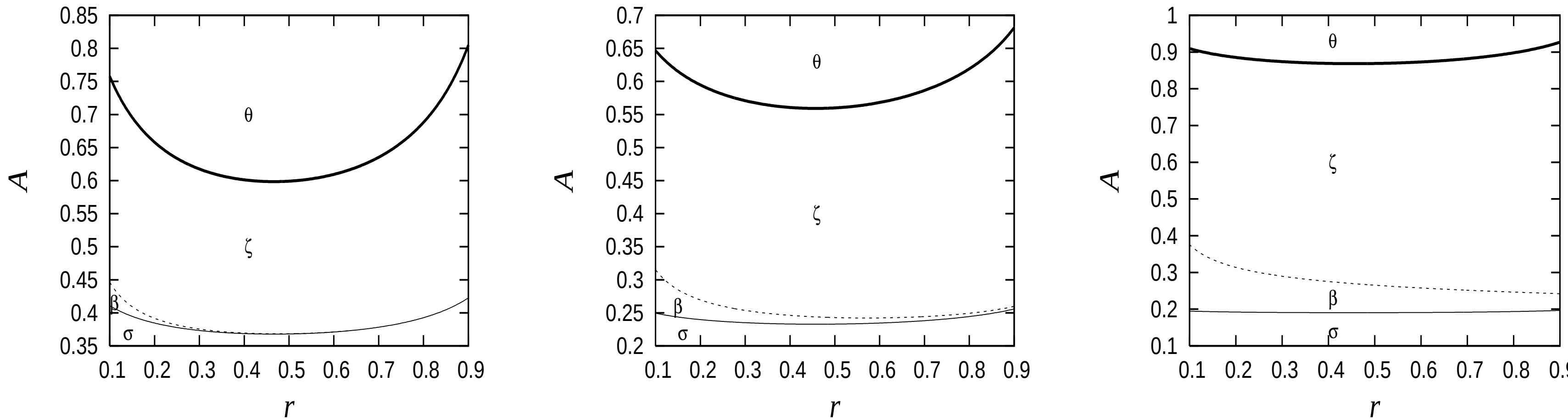


Left: Phase Diagram **Right:** $\tau_\pm$ vs. α for $A = 0.18, 0.20, 0.22$.

Key: A dynamically triggered spot self-replication instability is possible for α large enough (i.e. under-crowding instability).

K-Spot Patterns on a Ring in Unit Disk: I

Put spots at $x_j = r\,\exp(2\pi i j/K)$ for $j = 1, \ldots, K$, with $0 < r < 1$ in the unit disk. Fix $\varepsilon = 0.02$. **Phase Diagrams of A vs. Ring Radius r**

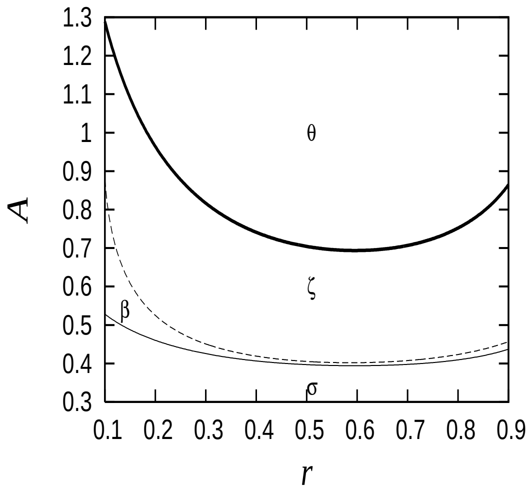


(c) $D = 0.2$, $K = 2$ (d) $D = 1.0$, $K = 2$ (e) $D = 5.0$, $K = 2$

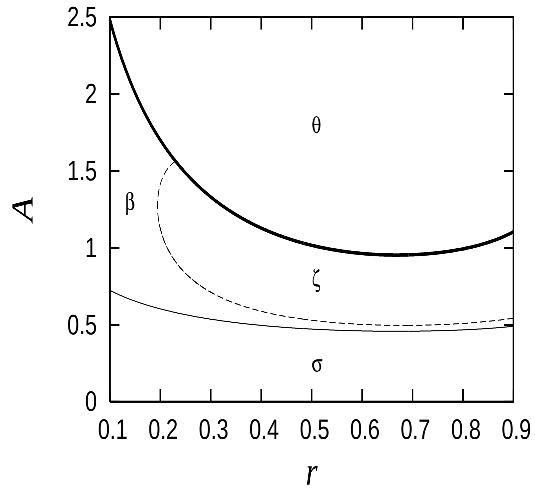
Note: Regime σ: no existence. β: unstable to competition. ζ: unstable to an oscillation if $\tau > \tau_H(r, A)$ (synchronous). θ: unstable to replication.

- **DAE Dynamics:** Equally-spaced spots on a ring, remain on a ring of slowly evolving radius, i.e. $r = r(\varepsilon^2 t)$.
- **Equilibrium:** Equilibrium ring radius coincides with minimum of $A_{\text{split}}(r)$ (upper curve).
- **Dynamically Triggered** spot self-replication and competition instabilities are clearly possible.

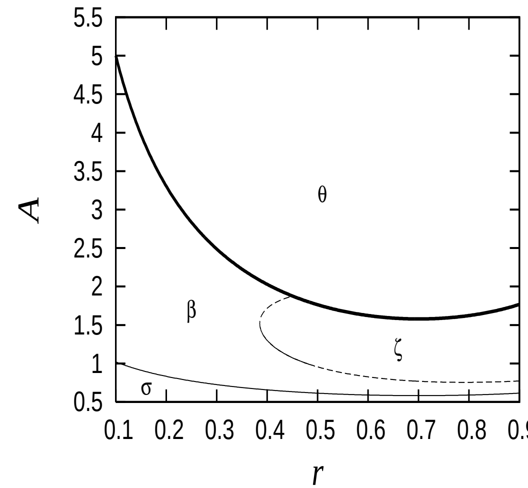
K-Spot Patterns on a Ring in Unit Disk: II



(f) $K = 4$, $D = 0.2$

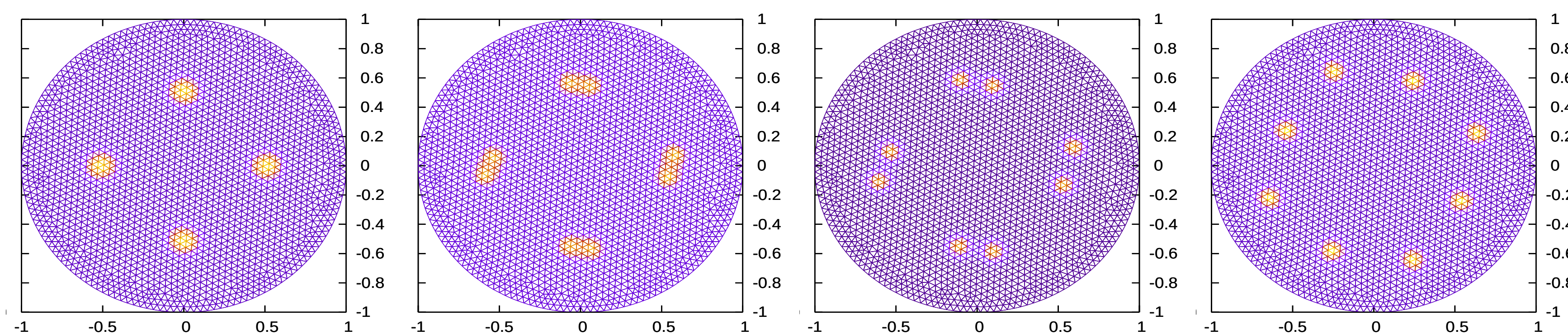


(g) $K = 8$, $D = 0.2$



(h) $K = 16$, $D = 0.2$

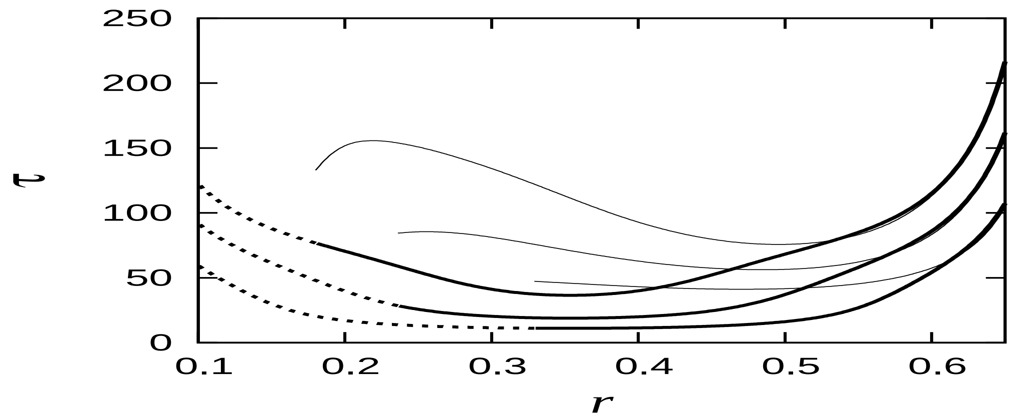
Ex: $K = 4$, $r(0) = 0.42$, $A = 0.7$. Predict: dynam. triggered instability.



Remark: Small eigenvalue instability associated with DAE dynamics if $K > K_c$ (similar to Eulerian point vortices on a ring or on equator).

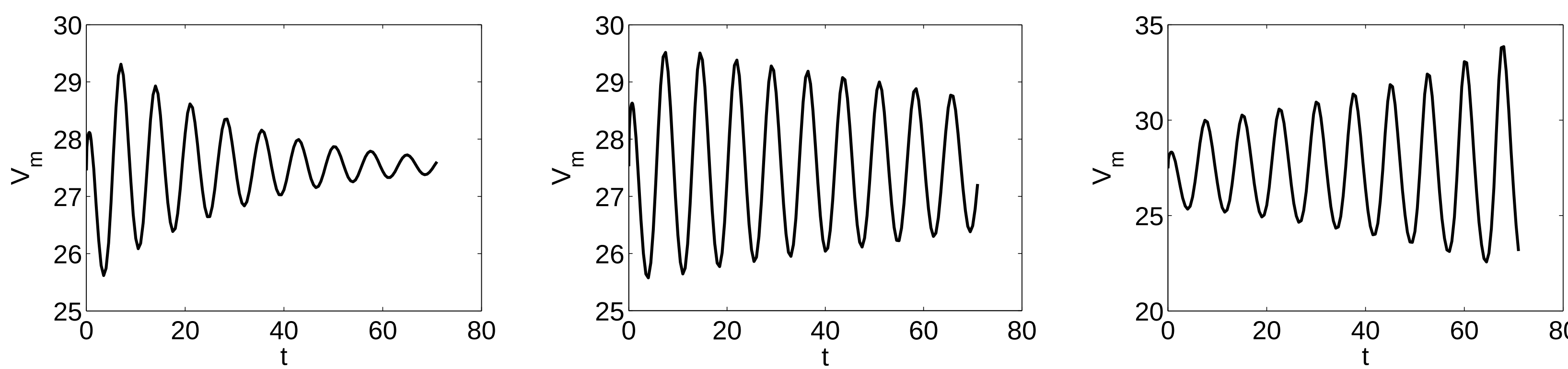
Oscillatory Instability: 4 Spots in Unit Square

Example: Put 4-spots along diagonals of the unit square at distance r from the center. Fix $D = 1$, $\varepsilon = 0.02$. Plot $\tau_H(r)$ for synchronous oscillation (heavy solid) and alternating-phase (light curves) for $A = 0.8$, $A = 0.9$, $A = 1.0$. Synchronous gives smallest τ_H. Note: Equilibrium at minimum value of $\tau_H(r)$. Hence, dynamically triggered oscillations are possible.



Example: Fix $r(0) = 0.35$, $A = 0.8$. Predict $\tau_H \approx 11.0$.

Left: $\tau = 10$ **Middle:** $\tau = 11$ **Right:** $\tau = 12$.

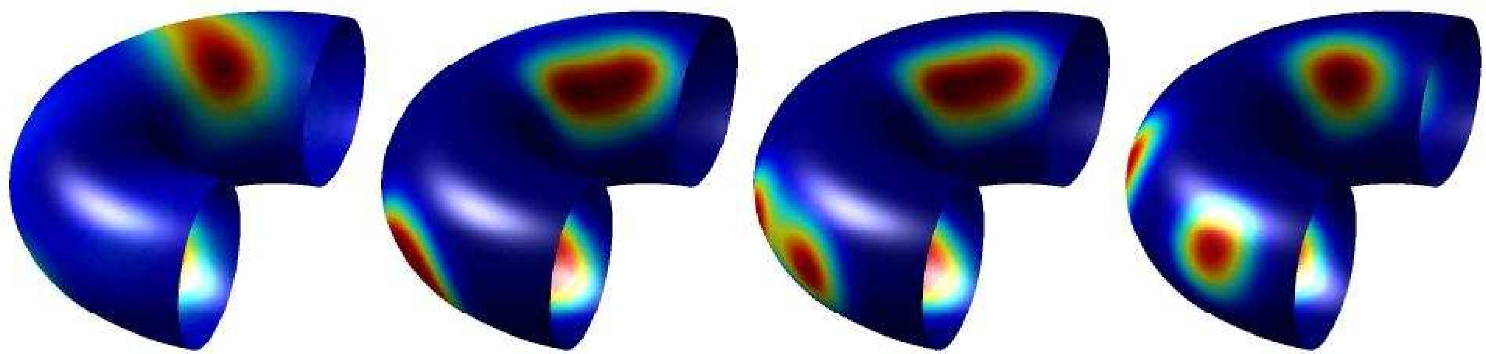


Open Issues and Further Directions: I

- **Rigor:** clearly a need for it
- **Universality:** Apply framework to (generic) RD systems to derive general principles for dynamics, stability, replication. (W. Chen, MJW)
- **Growing Domains:** Study delayed bifurcation effects and self-replication of spots on growing planar domains and on surface of a sphere (Ph.D thesis of Ignacio Rozada (UBC); ongoing).
- **Annihilation-Creation Attractor:** construct a “chaotic” attractor or “loop” for GS model composed of spot-replication events, leading to spot creation, followed by an over-crowding instability (spot-annihilation). (W. Chen, MJW).
- **Stability of Periodic Lattice Patterns in $\mathbb{R}^2$ for GS:** Need periodic G function for stability (Bloch representation); continuous spectrum etc..(Iron, Rumsey, MJW).
- **Cell Signalling:** Can localized compartments with ODE kinetics that are coupled together through a (slow) time-dependent (passive) diffusion process, trigger temporal oscillations in the compartments when no oscillations would otherwise be present? This is the mechanism of spot oscillations for GS model. (D. Coombs and Y. Nec (UBC)).

Open Issues and Further Directions: II

- **Patterns on Manifolds:** Pattern formation on manifolds, **where the geometry of the manifold influences localization**; equilibrium stripes on geodesics? dynamics of spots induced by Gaussian curvature? Spot replication on slowly evolving manifolds etc..Require properties of Green's functions on manifolds.



Schnakenburg model on a Manifold: S. Ruuth (JCP, 2008)

Key: New PDE numerical approaches "Closest Point Algorithms to Compute PDE's on Surfaces", by S. Ruuth (SFU) , C. McDonald (Oxford), allow for "routine" full numerical simulations to test any asymptotic theories.