Traps, Patches, Spots, and Stripes: Localized Solutions to Diffusive and Reaction-Diffusion Systems

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BIRS Meeting; Multi-Scale Analysis of Self-Organization in Biology

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Lecture II: Dynamics and Instabilities of Spots for Reaction-Diffusion Systems in Two-Dimensional Domains

Outline of the Talk

Overview: Localized Spot Solutions to RD systems

1. Particle-Like, Spot and/or Stripe Solutions to RD systems
2. Instability Types: Self-Replicating, Oscillatory, Over-Crowding or Annihilation, Breakup, Zigzag, etc..
3. Self-Replicating Spots (Laboratory and Numerical Evidence)
4. Theoretical approaches

Specific RD Systems in 2-D (Detailed Case Studies)

1. **GM Model:** Leading-order theory, based on ground-state solution to scalar PDE, Nonlocal eigenvalue problems, and critical points of Regular Part of Green's Functions
2. **Schnakenburg System:** Beyond leading-order theory: Self-Replication of Spots in 2-D; Dynamics of Collection of Spots (Main Focus)
3. **GS System:** Self-Replication, Oscillatory, and Annihilation Instabilities of Spots in 2-D. (Brief Summary) (Ph.D thesis work of Wan Chen).

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 $\Omega \in R^2$.

Semi-Strong Interaction Regime: $D = O(1)$ so that u is global.
Weak Interaction Regime: $D = O(\varepsilon^2)$ so that u is also localized.

Different Kinetics: (There is No Variational Structure)

- GM Model: (Gierer Meinhardt 1972; Meinhardt 1995).

$$g(u,v) = -v + v^p/u^q \qquad f(u,v) = -u + v^r/u^s\,.$$

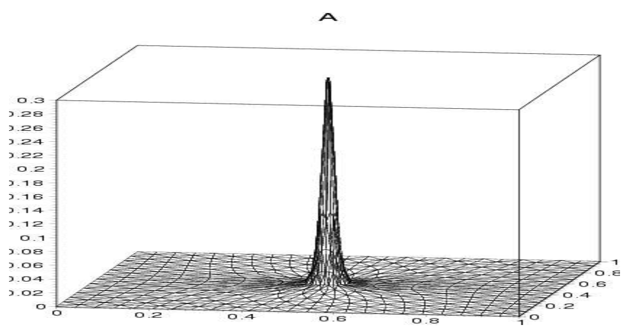
- GS Model: (Pearson, 1993, Swinney 1994, Nishiura et al. 1999)

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

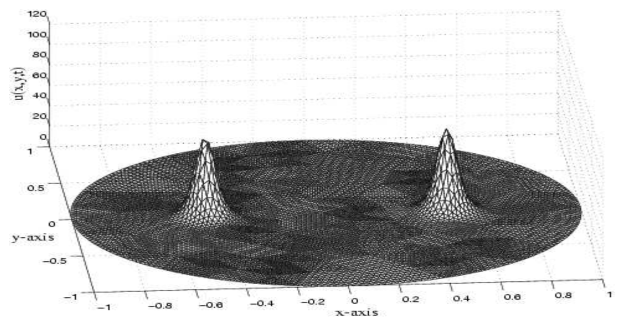
- Schnakenburg Model: $g(u,v) = -v + uv^2$ and $f(u,v) = a - uv^2$.

Spot Instabilities and Self-Replication

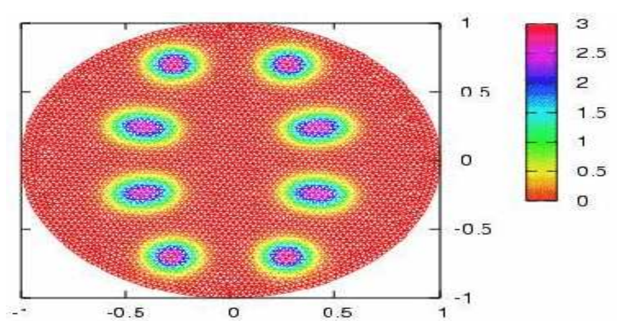
Snapshot of Phenomena for GM Model:



- The local profile for v is to leading-order approximated locally by a radially symmetric ground-state solution of $\Delta w - w + w^p = 0$. Particle-like solution to GM model.



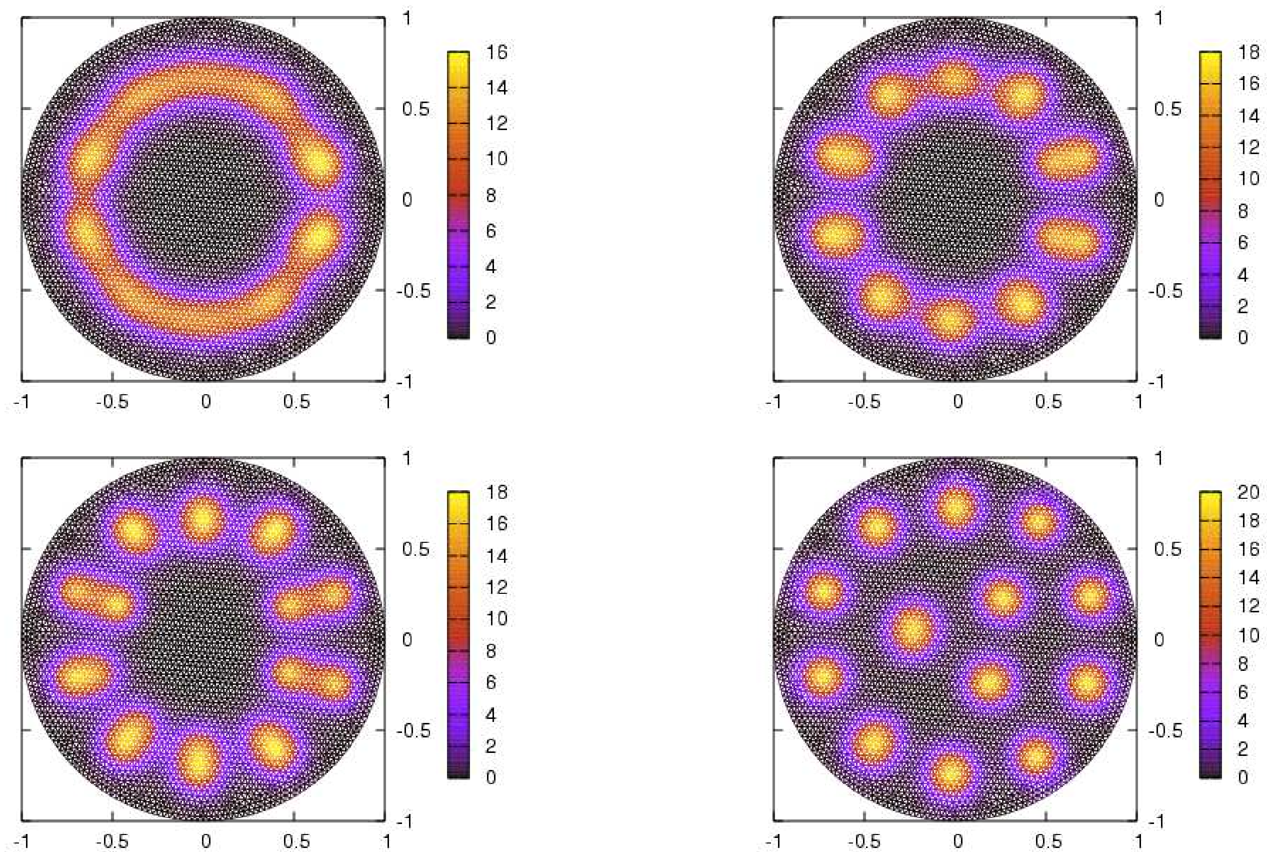
- **Semi-strong regime:** Slowly drifting spots can undergo sudden (fast) instabilities due to **dynamic bifurcations.** This leads to an overcrowding, or annihilation, instability (movie), or to oscillatory instabilities in the spot amplitude (movie)



- **Weak-interaction regime:** An isolated spot can undergo a repeated self-replication behavior, leading eventually to a Turing type pattern (movie).

Semi-Strong Regime: Breakup and Splitting

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 GS Model: Semi-strong regime.

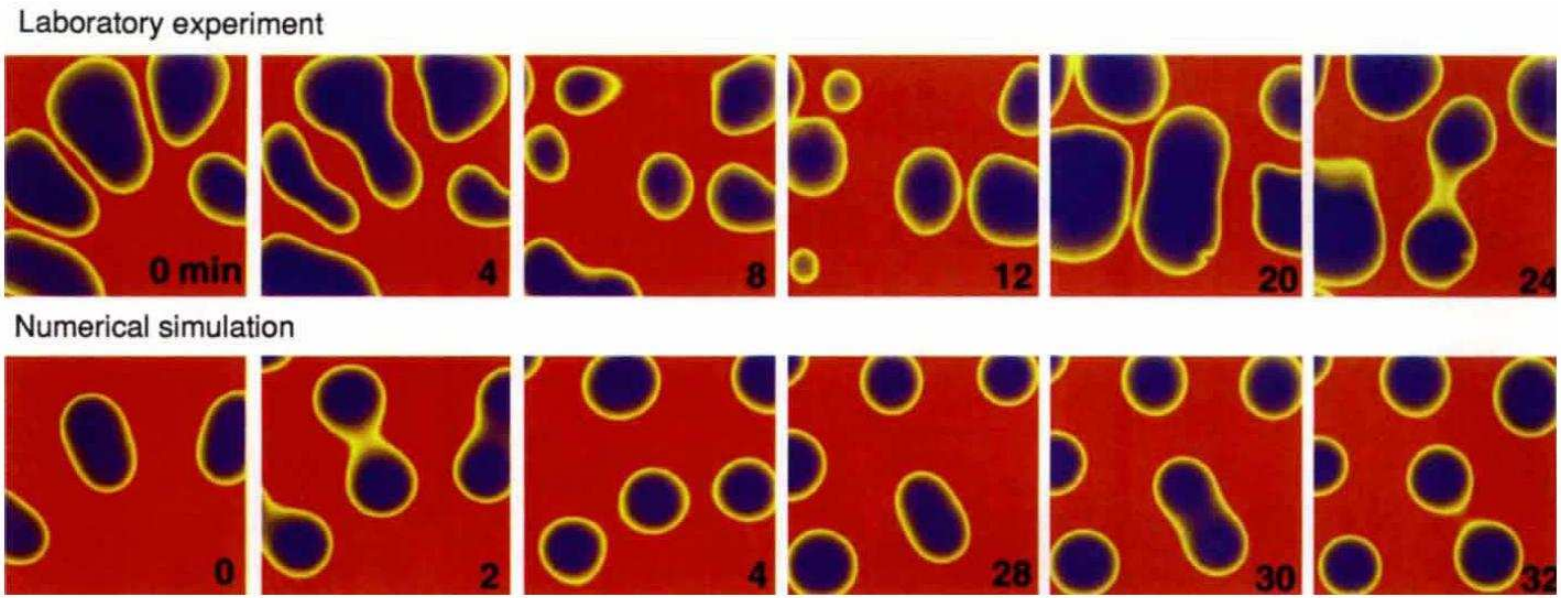


Ref: KWW, *Zigzag and Breakup Instabilities of Stripes and Rings....* Stud. Appl. Math., **116**, (2006), pp. 35–95.

Self-Replicating Spot Behavior: 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).

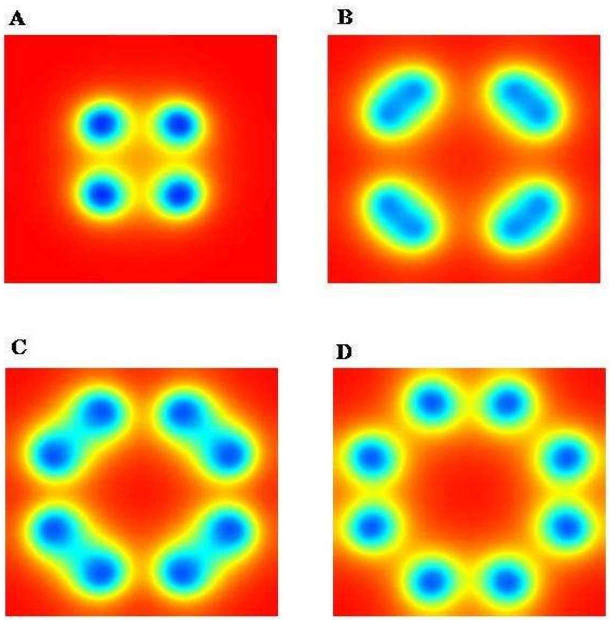


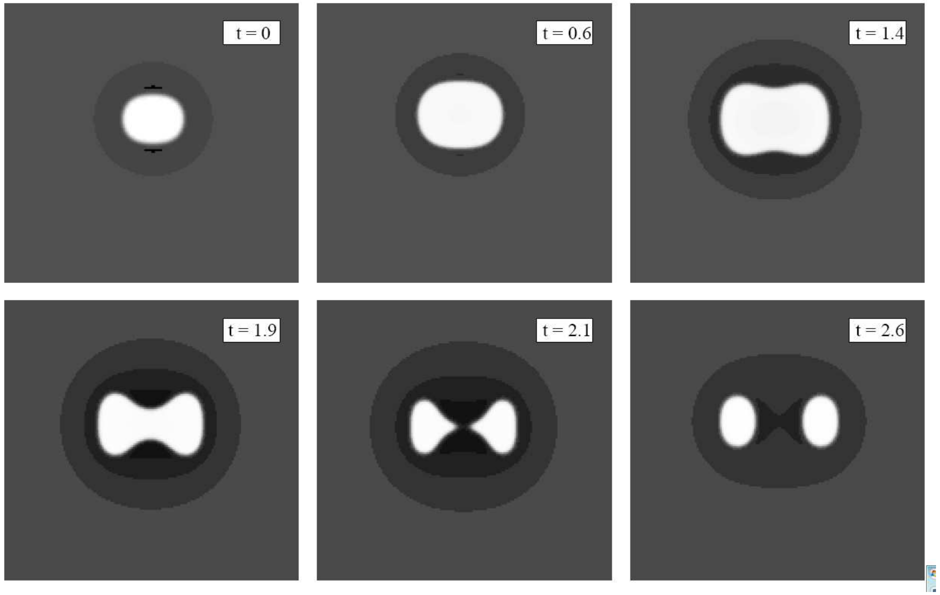
- A planar gas discharge system. (Astrov & Purwins, Phys. Lett. A, V. 283, (2001), pp. 349-354. Such systems often modeled by 3-component RD systems.

Self-Replicating Spot Behavior: II

Numerical evidence of spot-splitting

- Pearson, *Complex Patterns in a Simple System*, Science, **216**, pp. 189-192.
- Nishiura & Ueyama, *Spatial-Temporal Chaos in the Gray-Scott model*, Physica D, **150**, (3-4), (2001), pp. 137–152.
- Muratov & Osipov, *Scenarios of Domain Pattern Formation in Reaction-Diffusion Systems*, Phys. Rev. E, **54**, (1996), pp. 4860–4879.





Left: Pearson (1993).

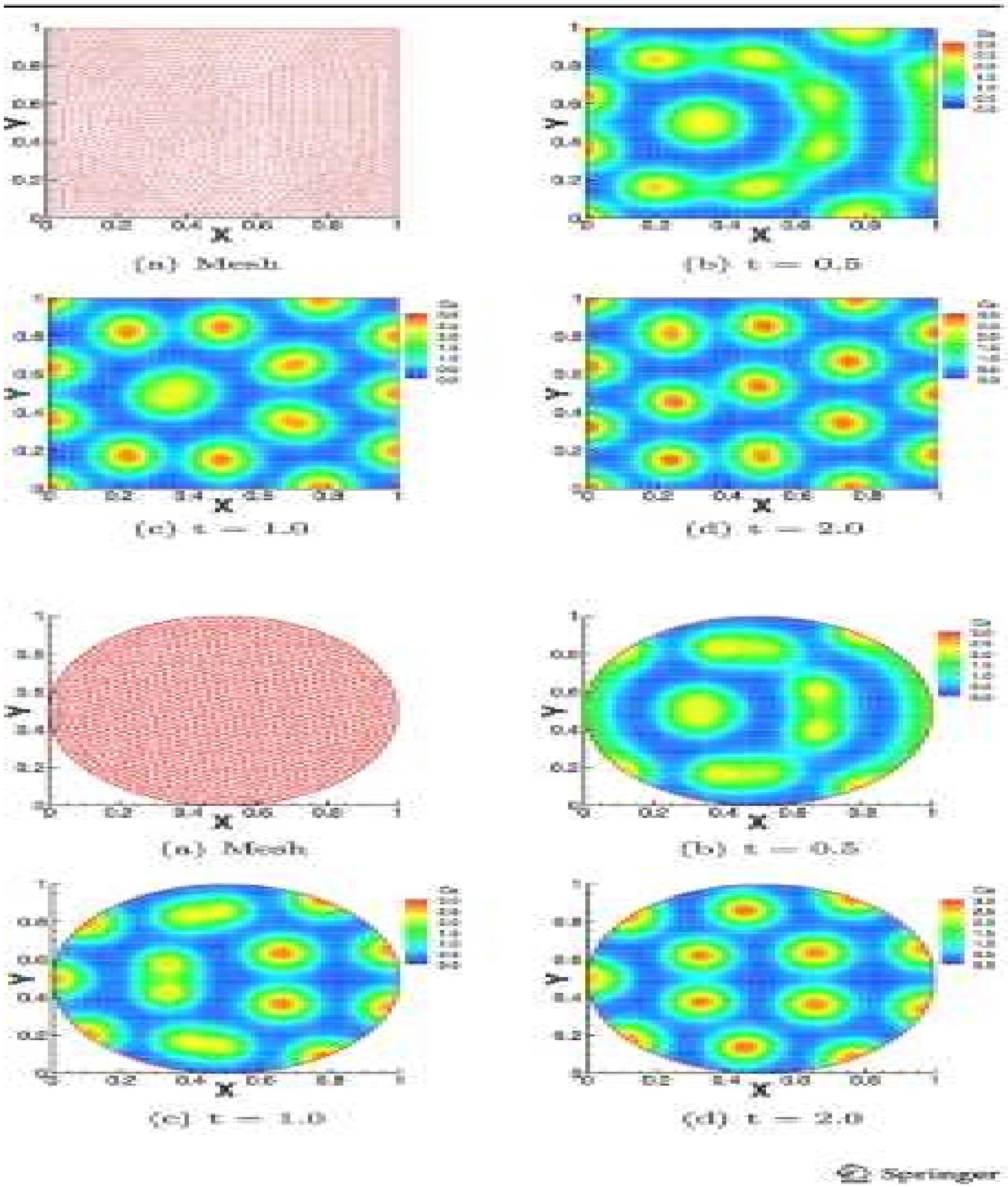
Right: Muratov and Osipov (1996).

Self-Replicating Spot Behavior: IV

Numerical evidence of spot-splitting

- Golovin, Matkowsky, Volpert, *Turing Patterns for the Brusselator with Superdiffusion*, SIAP, **68**, (2008), pp. 251–272.
- Glasner, *Spatially Localized Structures in Diblock Copolymer Mixtures*, SIAP, submitted, (2009).
- **Schnakenburg Model:**
  - J. Zhu et al., *Application of Discontinuous Galerkin Methods for RD Systems in Developmental Biology*, J. Sci. Comput., to appear, (2009).
  - A. Madvamuse, P. Maini, *Velocity-Induced Numerical Solutons of RD Systems on Continuously Growing Domains*, JCP, **225**, (2007), pp. 100-119.

Self-Replicating Spots for Schnakenburg



Self-replication of spots for the Schnakenburg model in the semi-strong regime in a 2-D domain (**Ref:** J. Zhu, J. Zhang, S. Newman, M. Alber, J. Sci. Comput., to appear, (2009)).

Theoretical Approaches: I

- **1) Turing Stability Analysis:** linearize RD around a spatially homogeneous steady state. Look for diffusion-driven instabilities (Turing 1952, and ubiquitous first step in RD models of math biology (e.g. J. Murray)).
- **2) Weakly Nonlinear Theory:** capture nonlinear terms in multi-scale perturbative way and derive normal form GL and CGL amplitude equations (Cross and Hohenberg, Knobloch, ...).
- **3) Localized Spot and Stripe patterns:**
  - Use singular perturbation techniques to construct quasi-steady pattern consisting of localized spots.
  - Dynamics of spots in terms of "collective" coordinates.
  - For stability, analyze singularly perturbed eigenvalue problems. Semi-strong interactions to leading-order in $-1/\log \varepsilon$ often lead to Nonlocal Eigenvalue Problems (NLEP).

Remarks on Approach 3):

- "Similar" to studying vortex dynamics (GL model of superconductivity)
- **Difficulty:** RD systems have no variational structure, and even leading-order NLEP problems are challenging to analyze.

Theoretical Approaches: III

Some Previous Analytical Work On Spike and Spot Patterns

- **1-D Theory: Spike Solutions to RD System**
  - Stability and dynamics of pulses for the GM and GS models in the semi-strong regime (Doelman, Kaper, Promisolow, Muratov, Osipov, Iron, MJW, Kolokolnikov, Chen, Wei),
  - 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), and the GM model (KWW, 2004).
- **2-D Theory: Spot Solutions to RD Systems**
  - Repulsive interactions of spots in weak interaction regime (Mimura, Ei, Ohta...)
  - NLEP stability theory for spot stability for GM and GS in semi-strong interaction regime (Wei-Winter, series of papers). NLEP problems arise from *leading-order* terms in infinite logarithmic expansion in ε.
  - One-Spot dynamics for GM (Chen, Kowalczyk, Kolokolnikov, MJW).

Largely Open: Give an analytical theory for self-replication of spots, dynamics of spots, and other instabilities (oscillatory and annihilation). Focus on semi-strong regime where analysis can be done.

Case Study: Older Results for GM Model I

The GM model in a 2-D bounded domain Ω, with $\varepsilon \ll 1$ is

$$v_t = \varepsilon^2 \Delta v - v + \frac{v^2}{u}, \qquad \tau u_t = D \triangle u - u + \varepsilon^{-2} v^2 .$$

Principal Result: *Provided that a stability condition on the spot profile is satisfied, then for $D \geq O(-\ln \varepsilon)$ and $\varepsilon \ll 1$ the spot dynamics is*

$$\frac{dx_0}{dt} \sim -4\pi\varepsilon^2 \left(\frac{1}{-\ln \varepsilon + 2\pi \frac{D}{|\Omega|}} \right) \nabla R_0 ,$$

where $R(x; x_0)$ is the regular part of the Neumann Green's function. (X. Chen and M. Kowalczyk (2003), T. Kolokolnikov and MJW (2003)).

Principal Result: (KW) *Provided that a stability condition on the spot profile is satisfied, then for $D = O(1)$ and $\varepsilon \to 0$ the dynamics of a spot satisfies*

$$\frac{dx_0}{dt} \sim -\frac{4\pi\varepsilon^2}{\ln(\frac{1}{\varepsilon}) + 2\pi R_{d0}} \nabla R_{d0} ,$$

where $R_d(x; x_0)$ is the regular part of the reduced wave G-function.

Case Study: Older Results for GM Model II

The Neumann Green's Function: $G(x;x_0)$ with regular part $R(x;x_0)$ satisfies

$$\Delta G = \frac{1}{|\Omega|} - \delta(x - x_0)\,, \quad x \in \Omega\,; \quad \partial_n G = 0 \quad x \in \partial\Omega\,; \ \int_\Omega G\, dx = 0\,,$$

$$G(x;x_0) = -\frac{1}{2\pi}\log|x - x_0| + R(x;x_0)\,; \quad \nabla R_0 \equiv \nabla R(x;x_0)|_{x=x_0}\,.$$

The Reduced-Wave Green's Function $G_d(x;x_0)$ with regular part $R_d(x;x_0)$

$$\Delta G_d - \frac{1}{D} G_d = -\delta(x - x_0)\,, \quad x \in \Omega\,; \quad \partial_n G_d = 0 \quad x \in \partial\Omega\,,$$

$$G_d(x;x_0) = -\frac{1}{2\pi}\log|x - x_0| + R_d(x;x_0)\,; \quad \nabla R_{d0} \equiv \nabla R_d(x;x_0)|_{x=x_0}\,.$$

Critical Points of R and R_d: In a symmetric dumbbell-shaped domain:

- For $D \ll 1$, R_d is determined in terms of the distance function. Hence, $\nabla R_{d0} = 0$ has a root in each lobe of a dumbbell.
- For $D \gg 1$, ∇R_{d0} can be approximated by ∇R_0, the Neumann regular part, which has a root only at the origin. (explain see below)
- So what happens to the roots as D is varied? (Bifurcation must occur)

Case Study: Older Results for GM Model III

Consider the Dirichlet Green's function H, with regular part R_h:

$$\Delta H = -\delta(x - x_0) \quad x \in \Omega\,, \quad H = 0\,, \quad x \in \partial\Omega\,,$$

$$H(x, x_0) = -\frac{1}{2\pi} \log|x - x_0| + R_h(x; x_0)\,, \quad \nabla R_{h0} \equiv \nabla R_h(x, x_0)|_{x=x_0}\,.$$

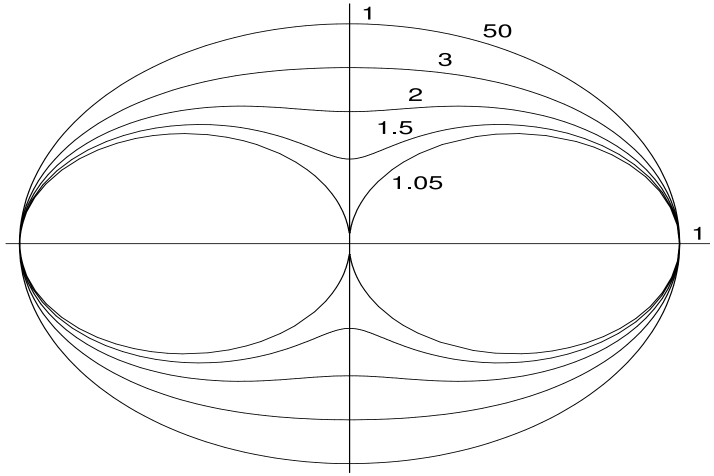
- For a strictly convex domain Ω, R_{h0} is strictly convex, and thus there is a unique root to $\nabla R_{h0} = 0$. (B. Gustafsson, Duke J. Math (1990), Caffarelli and Friedman, Duke Math J. (1985)).
- ∇R_{h0} can be found for certain mappings $f(z)$ of the unit disk as

$$f^{'}(z_0)\nabla R_{h0} = -\frac{1}{2\pi}\left(\frac{z_0}{1 - |z_0|^2} + \frac{f^{''}(\overline{z}_0)}{2f^{'}(\overline{z}_0)}\right)\,.$$

- Let B be the unit disk, and $f(z; a) = \frac{(1-a^2)z}{z^2-a^2}$. Then $f(B)$ is a symmetric but nonconvex dumbbell-shaped domain for $1 < a < 1 + \sqrt{2}$. Using the formula above, Gustafson (1990) proved that $\nabla R_{h0} = 0$ has three roots when $1 < a < \sqrt{3}$.
- One can derive a complex variable formula for the gradient of the regular part of the Neumann Green's function (Ref: KW, 2003 EJAM).

Case Study: Older Results for GM Model IV

Example: Let $f(z;a) = \frac{(1-a^2)z}{z^2-a^2}$; so $f(B)$ is nonconvex for $1 < a < 1+\sqrt{3}$. For any $a > 1$, the complex variable formula can be used to show that $\nabla R_0 = 0$ has exactly one root at $z = 0$. This is qualitatively different than for the Dirichlet problem.



Remark 1: Recall that the principal eigenvalue λ_1 of the Laplacian with one localized trap of radius ε

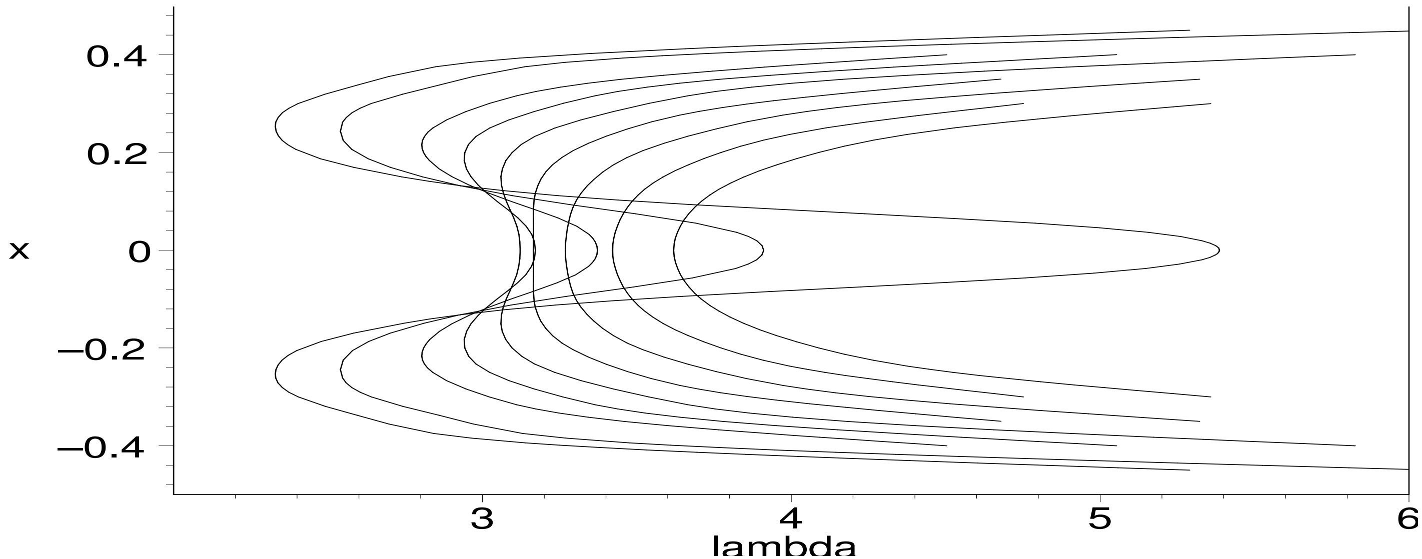
$$\lambda_1 \sim \frac{2\pi\nu}{|\Omega|} - \frac{4\pi^2\nu^2}{|\Omega|} R(x_0; x_0)\,, \quad \nu = -1/\log\varepsilon\,.$$

Thus, λ_1 is maximized for a symmetric dumbell-shaped domain by putting the trap at the center of the neck (which is intuitively clear).

Case Study: Older Results for GM Model V

Remark 2: In non-symmetric dumbell-shaped domains $\nabla R_0 = 0$ for Neumann G-function can have multiple roots (Kolokolnikov, Titcombe, MJW, EJAM, 2004).

Reduced-Wave G-Function: Now use a BEM scheme to compute the roots of $\nabla R_{d0} = 0$ for the same class of mappings of the unit disk. Plot the zeroes of $\nabla R_{d0} = 0$ along the real axis x versus $\lambda \equiv D^{-1/2}$. There is a subcritical pitchfork bifurcation for two nearly disjoint circles (a near one), and a supercritical pitchfork when $a \gg 1$. (Open: Rigorous Theory??).



Case Study: Older Results for GM Model VI

Theorem: (Winter Wei, (2001) JNS) *For $\tau = 0$, $\varepsilon \to 0$, and $D \gg O(-\ln \varepsilon)$, an N-spot equilibrium solution is stable on an $O(1)$ time scale iff*

$$D < D_N \sim -\frac{|\Omega| \ln \varepsilon}{2\pi N} .$$

Analysis based on NLEP problem, for inner region with $\rho = |y|$

$$\Delta\Phi - \Phi + 2w\Phi - \chi w^2 \frac{\int_{\mathbb{R}^2} w\Phi \, dy}{\int_{\mathbb{R}^2} w^2 \, dy} = \lambda\Phi ,$$

where $\Delta w - w + w^2 = 0$ is the scalar ground-state solution describing the spot profile.

- Leading-order theory predicts that D_N is independent of spot locations x_i, $i = 1, \ldots, N$.
- Need higher order terms in the logarithmic series in ν for D_N similar to mean first passage time problems in 2-D with traps. We suggest

$$D_N \sim \frac{-|\Omega| \ln \varepsilon + F(x_1, \ldots, x_N)}{2\pi N} + O(\nu^{-1}) , \quad \nu \equiv -1/\ln \varepsilon .$$

Detailed Case Study: Schnakenburg Model

Schnakenburg Model: in a 2-D domain Ω consider

$$v_t = \varepsilon^2 \Delta v - v + uv^2 \,, \qquad \varepsilon^2 u_t = D \Delta u + a - \varepsilon^{-2} uv^2 \,,$$
$$\partial_n u = \partial_n v = 0 \,, \quad x \in \partial\Omega \,.$$

Here $0 < \varepsilon \ll 1$, and the two parameters are $D > 0$, and $a > 0$.

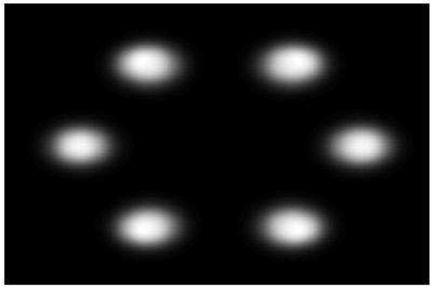
Ref: Kolokolnikov, Ward, Wei, *Spot Self-Replication and Dynamics for the Schnakenburg Model...* J. Nonl. Sci., 19, (2009), pp. 1–56.

Detailed Outline: Spot Dynamics and Spot Self-Replication

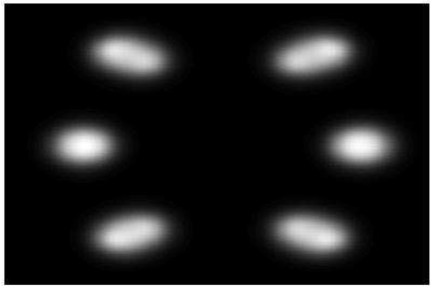
- **Quasi-Equilibria:** Asymptotic construction (summing log expansion).
- **Slow Dynamics:** Derive DAE system for the evolution of K spots.
- **Spot-Splitting Instability**: peanut-splitting and the splitting direction.
- **Numerical Confirmation of Asymptotic Theory:** Unit Square and unit disk.

Schnakenburg Model: Numerical Simulations

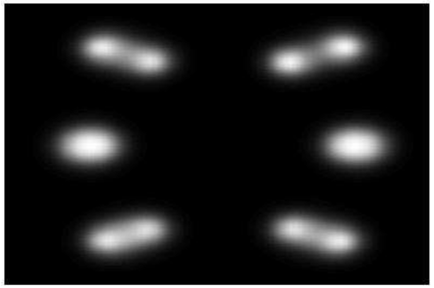
Example: $\Omega = [0,1]^2$, $\varepsilon = 0.02$, $a = 51$, $D = 0.1$. (movie 1).



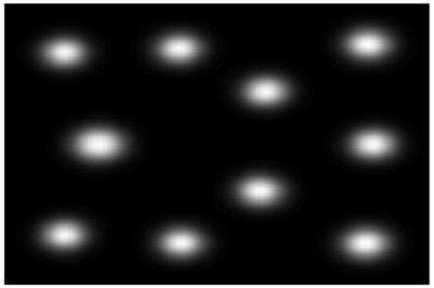
$t = 4.0$



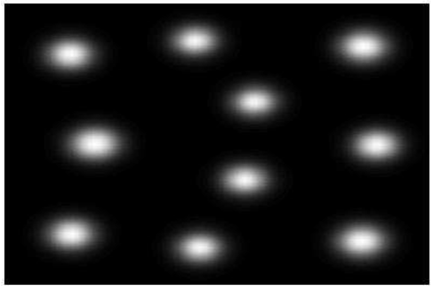
$t = 25.5$



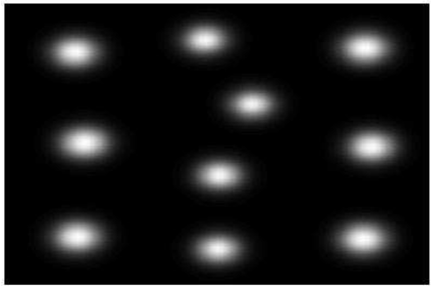
$t = 40.3.$



$t = 280.3$



$t = 460.3$



$t = 940.3.$

- Detailed mechanism for spot splitting?
- Why do some spots split and not others?
- Characterize the dynamics of the spots after splitting?

The Quasi-Equilibrium Solution: I

Asymptotic Construction of a One-Spot Pattern

Inner Region: near the spot location $x_0 \in \Omega$ introduce $\mathcal{V}(y)$ and $\mathcal{U}(y)$ by

$$u = \frac{1}{\sqrt{D}}\mathcal{U}\,, \quad v = \sqrt{D}\mathcal{V}\,, \quad y = \varepsilon^{-1}(x - x_0)\,, \quad x_0 = x_0(\varepsilon^2 t)\,.$$

To leading order, $\mathcal{U} \sim U(\rho)$ and $\mathcal{V} \sim V(\rho)$ (radially symmetric) with $\rho = |y|$.

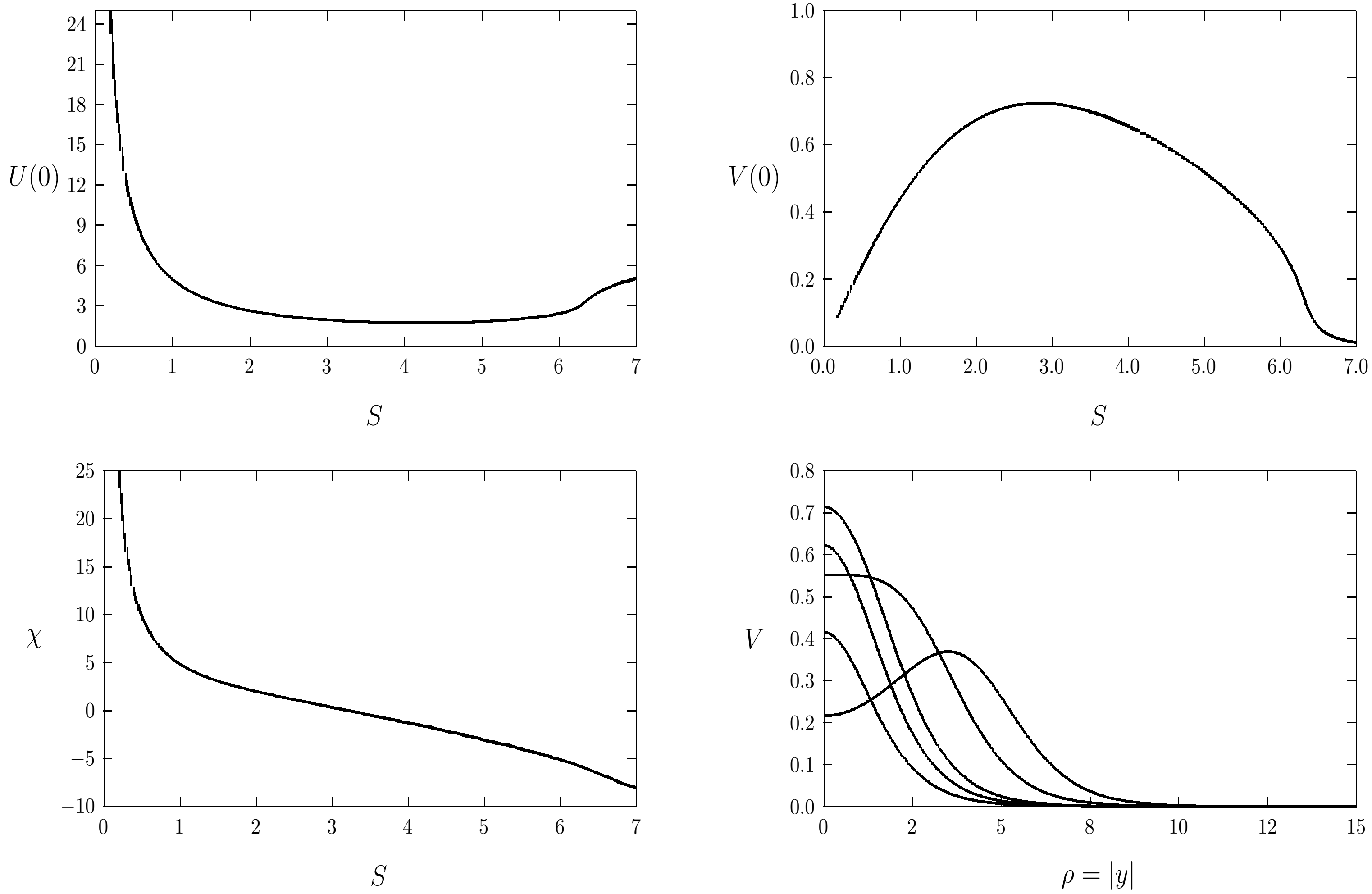
This yields the **coupled core problem** with $U'(0) = V'(0) = 0$, where:

$$V_{\rho\rho} + \frac{1}{\rho}V_\rho - V + UV^2 = 0\,, \quad U_{\rho\rho} + \frac{1}{\rho}U_\rho - UV^2 = 0\,, \qquad 0 < \rho < \infty\,,$$
$$V \to 0\,, \qquad U \sim S\log\rho + \chi(S) + o(1)\,, \quad \text{as} \quad \rho \to \infty\,.$$

- Here $S > 0$ is called the "source strength" and is a parameter to be determined upon matching to an outer solution.
- The nonlinear function $\chi(S)$ must be computed numerically.
- Thus, the "ground-state problem" is a coupled set of BVP, in contrast to approach based on NLEP theory.

The Quasi-Equilibrium Solution: II

Plots of the Numerical Solution to the Core Problem:



Lower left figure: The key relation is the $\chi = \chi(S)$ curve

The Quasi-Equilibrium Solution: III

Outer Region: $v \ll 1$ and $\varepsilon^{-2} u v^2 \to 2\pi\sqrt{D} S \delta(x - x_0)$. Hence,

$$\Delta u = -\frac{a}{D} + \frac{2\pi}{\sqrt{D}} S\,\delta(x - x_0)\,, \quad x \in \Omega\,; \quad \partial_n u = 0\,, \quad x \in \partial\Omega\,,$$

$$u \sim \frac{1}{\sqrt{D}} \left[S \log|x - x_0| + \chi(S) + \frac{S}{\nu} \right] \quad \text{as} \quad x \to x_0\,, \quad \nu \equiv -1/\log\varepsilon\,.$$

Key Point: the regular part of this singularity structure is **specified** and was obtained from matching to the **inner core solution.**

- Divergence theorem yields S (specifying core solution U and V) as

$$S = \frac{a|\Omega|}{2\pi\sqrt{D}}\,.$$

- The outer solution is given uniquely in terms of the Neumann G-function and its regular part by

$$u(x) = -\frac{2\pi}{\sqrt{D}} \left(S G(x; x_0) + u_c \right)\,,$$

where $\quad S + 2\pi\nu S R(x_0; x_0) + \nu\chi(S) = -2\pi\nu u_c\,, \qquad \nu \equiv -1/\log\varepsilon\,.$

The Quasi-Equilibrium Solution: IV

Remarks On Asymptotic Construction:

- G, its regular part R, and their gradients, can be calculated for different Ω. (Simple formulae for a disk; more difficult for a rectangle where Ewald-type summation is needed).
- Construction yields a quasi-equilibrium solution for any "frozen" x_0.
- No rigorous existence theory for solutions to the coupled core problem.
- The error is smaller than any power of $\nu = -1/\log \varepsilon$. Therefore, in effect, we have "summed" all the logarithmic terms.
- Related infinite log expansions: eigenvalue of the Laplacian in a domain with localized traps, slow viscous flow over a cylinder, etc.
- For the trap problems the inner problem is linear and in 2-D we must solve

$$\Delta_y U = 0\,, \quad y \notin \Omega_1\,; \quad U = 0\,, \quad y \in \partial\Omega_1\,,$$
$$U \sim \log|y| - \log d\,, \quad |y| \to \infty\,,$$

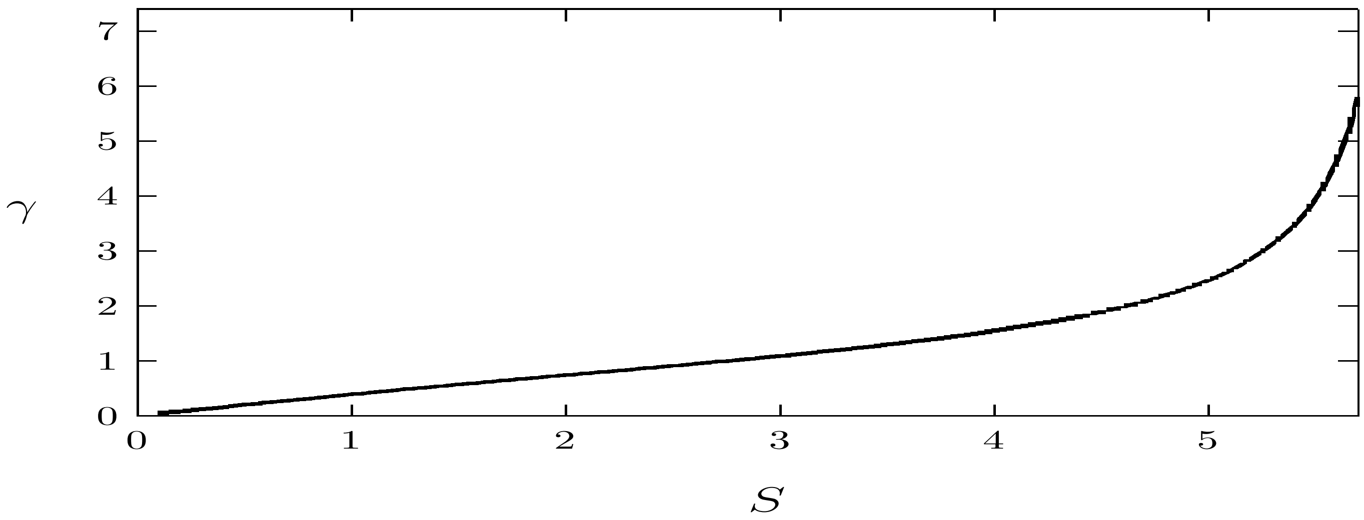
where d is the logarithmic capacitance. Our inner nonlinear core problem yields $U \sim S \log|y| + \chi(S)$ as $|y| \to \infty$.

The One-Spot Dynamics: I

Principal Result: *Provided that the one-spot profile is stable, the slow dynamics of a one-spot solution satisfies the gradient flow*

$$\frac{dx_0}{dt} \sim -2\pi\varepsilon^2 \gamma(S) S \ \nabla R(x_0; x_0) \,.$$

- Here $\gamma(S) > 0$ is determined from the **inner problem** by a solvability condition, and is computed numerically
- **Key:** a stable equilibrium occurs at a minimum point of $R(x_0; x_0)$.
- Plot of numerically computed $\gamma(S)$:



The Stability of a One-Spot Solution: I

We seek fast $\mathcal{O}(1)$ time-scale instabilities relative to slow time-scale of x_0.

Let $u = u_e + e^{\lambda t}\eta$ and $v = v_e + e^{\lambda t}\phi$. In the **inner region** we introduce the local angular mode $m = 0, 2, 3, \ldots$ by

$$\eta = \frac{1}{D} e^{im\theta} N(\rho) \,, \quad \phi = e^{im\theta}\Phi(\rho) \,, \quad \rho = |y| \,, \qquad y = \varepsilon^{-1}(x - x_0) \,.$$

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

$$\mathcal{L}_m \Phi - \Phi + 2UV\Phi + V^2 N = \lambda \Phi \,, \qquad \mathcal{L}_m N - 2UV\Phi - V^2 N = 0 \,,$$

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

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

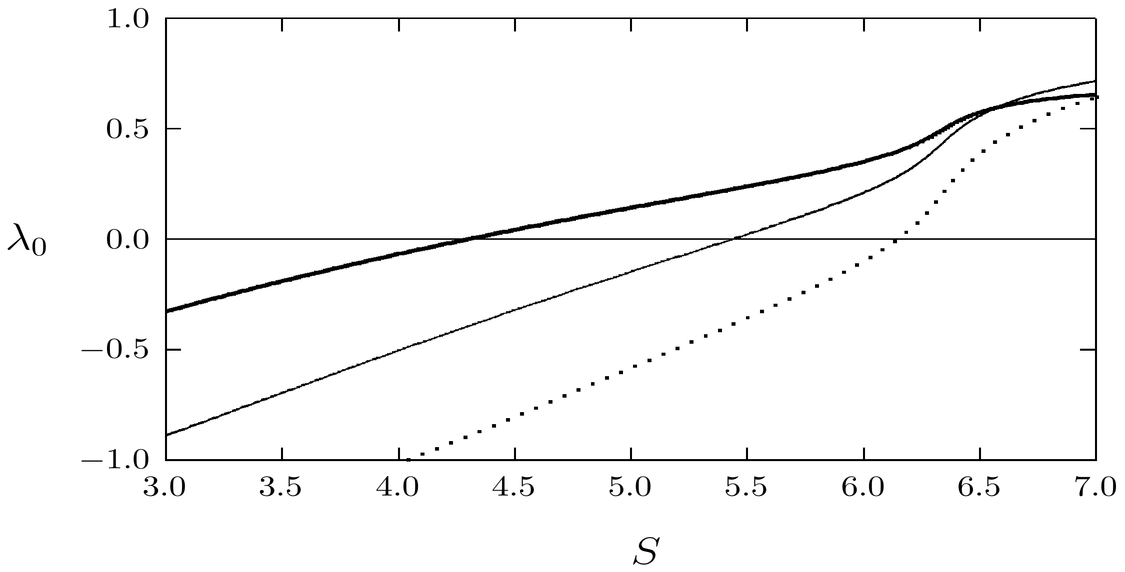
- U and V are computed from the core problem and depend on S.
- **Key Point:** This is a two-component eigenvalue problem, in contrast to the scalar problem of NLEP theory. Hence, there is no ordering principle for eigenvalues wrt number of nodal lines of eigenfunctions.

The Stability of a One-Spot Solution: II

Definition of Thresholds: Let $\lambda_0(S, m)$ denote the eigenvalue with the largest real part, with Σ_m being the value of S such that Re$\lambda_0(\Sigma_m, m) = 0$.

The Modes $m \geq 2$: We must impose $N \sim \rho^{-2}$ as $\rho \to \infty$. We compute

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

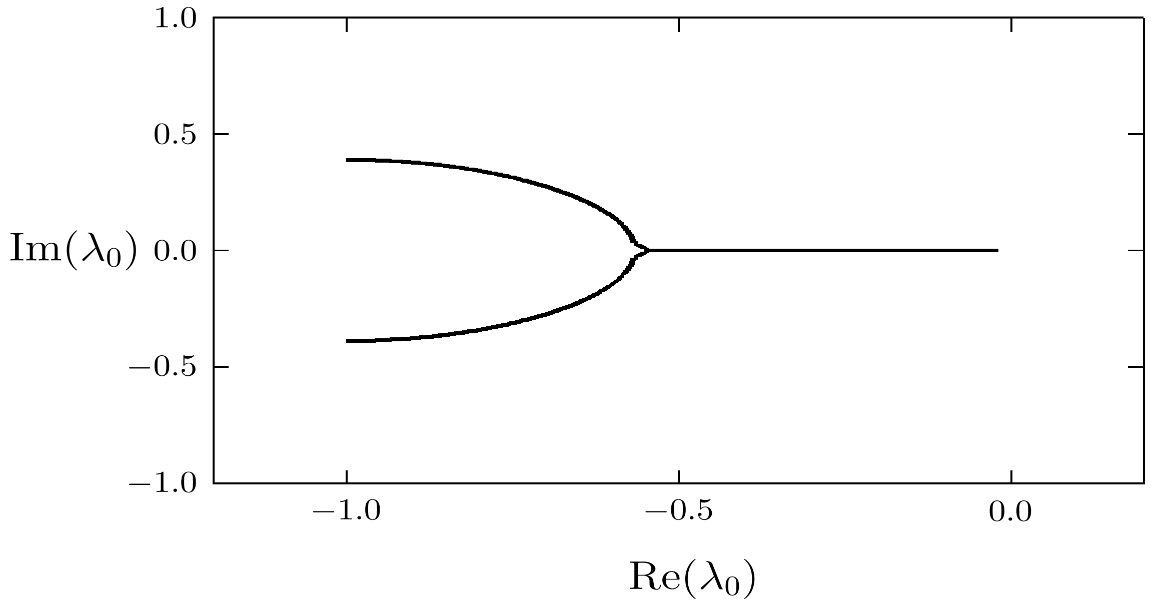


Key points:

- The peanut-splitting instability $m = 2$ is dominant.
- Since $N \to 0$ as $\rho \to \infty$, this is a local instability

The Stability of a One-Spot Solution: III

The Mode $m = 0$: Must allow for N to behave logarithmically at infinity. Hence, it must be matched to an outer solution. For our one-spot solution, this matching shows that N must be bounded as $\rho \to \infty$.



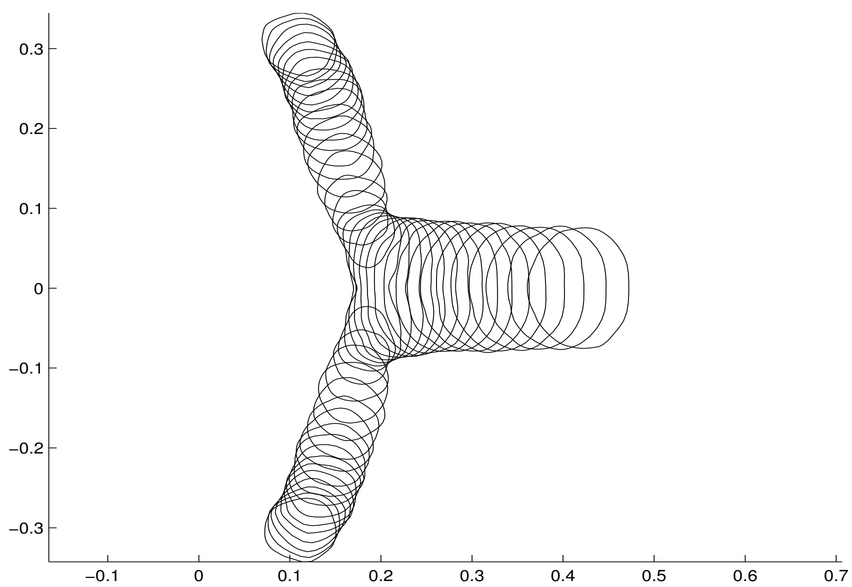
Caption: eigenvalue path as a function of S

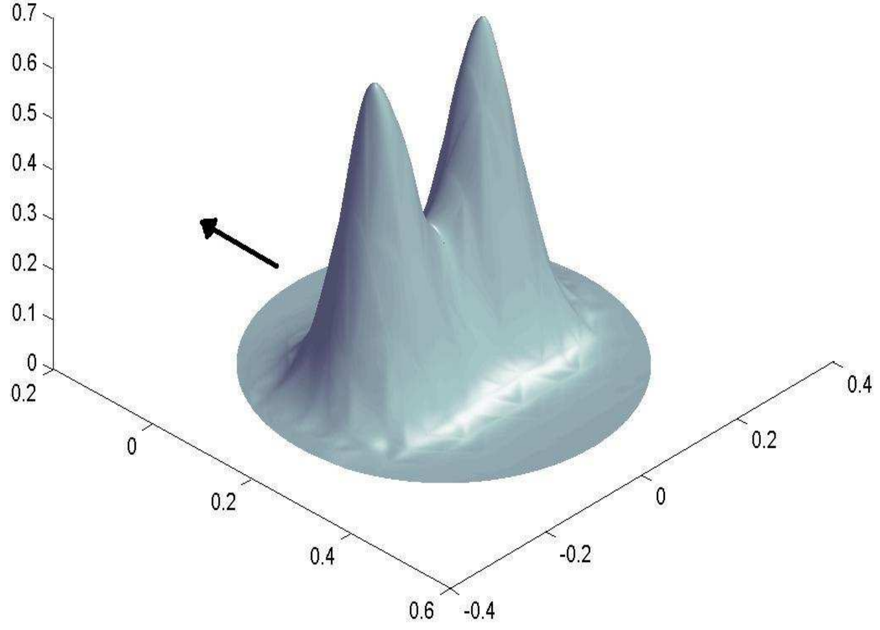
Key Point: Numerical computations show that we have stability wrt this mode at least up to $S = 7.8$.

The Direction of Splitting

- For $S \approx \Sigma_2$, the linearization of the core problem has an approximate four-dimensional null-space (two translation and splitting modes).
- By deriving a certain solvability condition (center manifold-type reduction), we show that for a one-spot solution splitting occurs in a direction perpendicular to the motion when $\varepsilon \ll 1$.

Spot-Splitting in the Unit Disk: $x_0(0) = (0.5, 0.0)$, $\varepsilon = 0.03$, $D = 1$, and $a = 8.8$. 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.





The DAE System for a K-Spot Pattern: I

Collective Slow Coordinates: S_j, x_j, for $j = 1, \ldots, K$.

Principal Result: (DAE System): *For "frozen" spot locations x_j, the source strengths S_j and u_c satisfy the nonlinear algebraic system*

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

$$\sum_{j=1}^{K} S_j = \frac{a|\Omega|}{2\pi\sqrt{D}} \,, \qquad \nu \equiv \frac{-1}{\log \varepsilon} \,.$$

The spot locations x_j, with speed $O(\varepsilon^2)$, satisfy

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

Here $G_{j,i} \equiv G(x_j; x_i)$ and $R_{j,j} \equiv R(x_j; x_j)$ (Neumann G-function).

The DAE System II: Qualitative Comments

- **Vortices in GL Theory:** some similarities for the law of motion.
- **Spot-Splitting Criterion:** For $D = O(1)$ and $K \geq 1$ the q. e. solution is stable wrt the local angular modes $m \geq 2$ iff $S_j < \Sigma_2 \approx 4.303$ for all $j = 1, \ldots, K$. The J^{th} spot is unstable to the $m = 2$ peanut-splitting mode when $S_J > \Sigma_2$, which triggers a nonlinear spot self-replication process. **Note: asymptotically no inter-spot coupling when $m \geq 2$.**
- **Stability to Locally Radially Symmetric Fluctuations:** For $D = O(1)$, and to leading order in ν, a K-spot q. e. solution with $K > 1$ is stable wrt $m = 0$. A one-spot solution is always stable wrt $m = 0$.
- **NLEP theory when $\mathbf{D = 0(\nu^{-1}) \gg 1}$:** Yields a scalar inner eigenvalue problem, so that the $m = 2$ mode is always stable. For $K \geq 2$, the $m = 0$ mode is stable only when

$$D \leq D_{0K} \equiv \frac{a^2 |\Omega|^2 \nu^{-1}}{4\pi^2 K^2 b_0} ; \quad b_0 \equiv \int_0^\infty \rho \left[w(\rho) \right]^2 \, d\rho \, .$$

- **Universality:** For other RD systems, similar DAE systems but with other $\gamma(S)$ and $\chi(S)$ (from other core problems), and possibly with other G-functions (such as reduced-wave G-function), can be derived.

Comparison: Asymptotics with Full Numerics

Asymptotic Theory

- **Inner:** Compute $\gamma(S)$ and $\chi(S)$ from core problem at discrete points in S. Then, interpolate with a spline.
- **Domain:** Calculate G, its regular part R, and gradients of G, R. This can be done analytically for the unit ball and the square.
- Solve DAE system numerically using Newton's method for nonlinear algebraic part, and a Runge-Kutta ODE solver for the dynamics.
- For special geometries, the algebraic part of the DAE system can be solved analytically (ring patterns in a disk).

Full Numerics

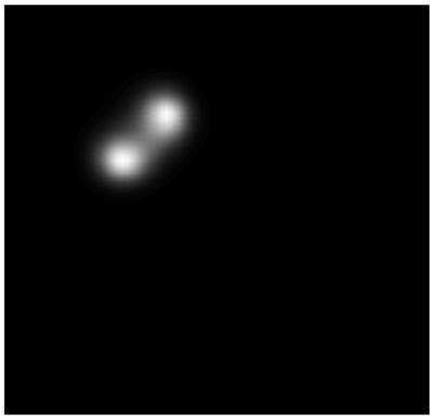
- Adaptive grid finite-difference code VLUGR2 (P. Zegeling, J.Blom, J. Verwer) to compute solutions in a square. Use finite-element code of W. Sun (U. Calgary) for a disk. "Prepared" initial data:

$$v = \sqrt{D} \sum_{j=1}^{K} v_j \text{sech}^2 \left(\frac{|x - x_j|}{2\varepsilon} \right) , \quad u = -\frac{2\pi}{\sqrt{D}} \left(\sum_{j=1}^{K} S_j G(x; x_j) + u_c \right) .$$

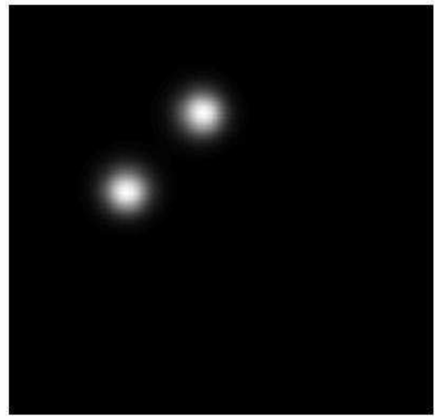
- Find the location of maxima of v on the computational grid

Numerical Validation for 1-Spot Solution

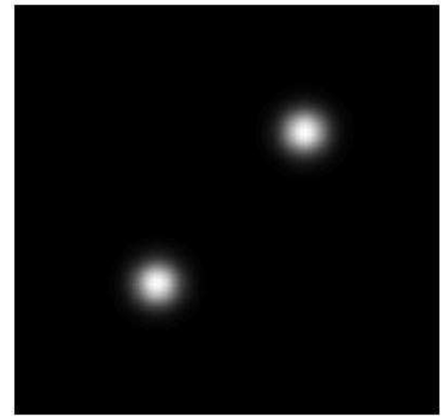
Splitting of One Spot: Let $\Omega = [0,1]^2$ and fix $\varepsilon = 0.02$, $x_0 = (0.2, 0.8)$, $a = 10$, and $D = 0.1$. Then, $S \approx 5.03 > \Sigma_2$. We predict a spot-splitting event beginning at $t = 0$. The growth rate is $\lambda_0(S, 2) \approx 0.15$. (movie)



$t = 23.6$



$t = 40.2$



$t = 322.7$.

- For $\varepsilon = .02$, full numerics gives a threshold in $4.15 < S < 4.28$.
- Splitting occurs in direction perpendicular to motion.
- In a slowly growing square $\Omega = [0, L]^2$, we predict spot-splitting when

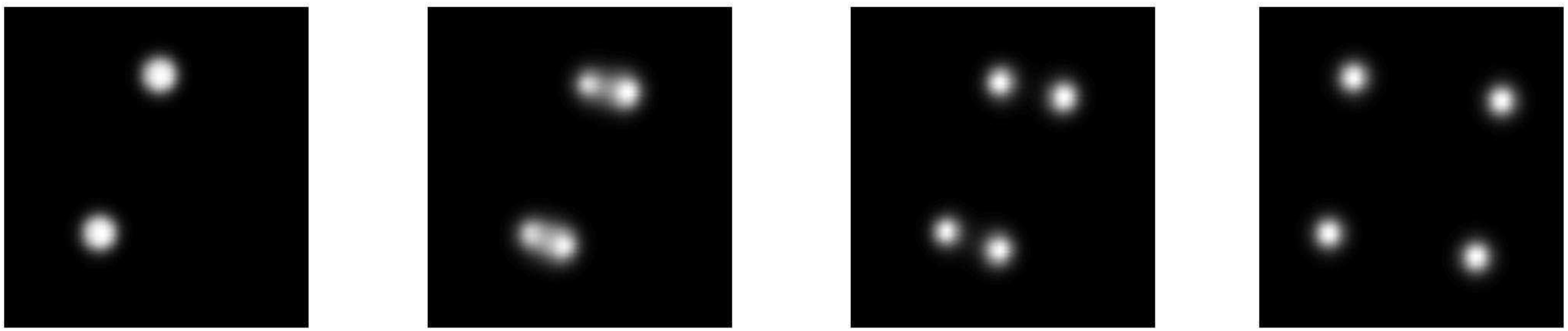
$$L > L_1 = \left(\frac{2\pi\sqrt{D}\Sigma_2}{a} \right)^{1/2} .$$

Numerical Validation, 2-Spot Solutions: I

Let $\Omega = [0,1]^2$. Fix $\varepsilon = 0.02$, $x_1(0) = (0.3, 0.3)$, $a = 18$, and $D = 0.1$.

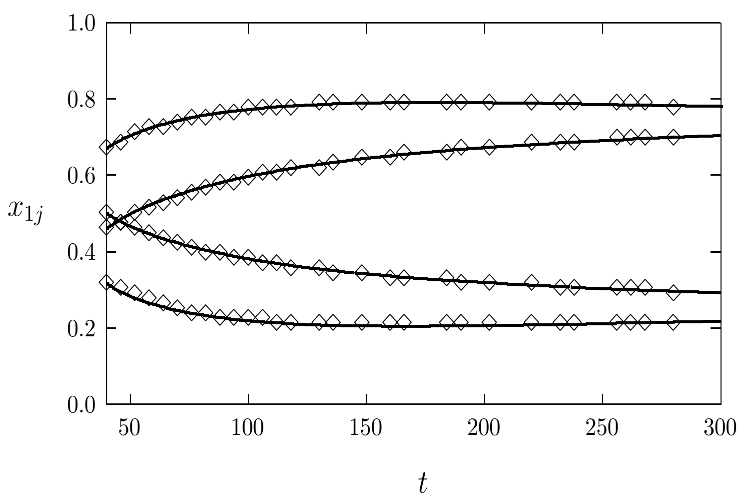
We only only vary $x_2(0)$, the initial location of the second spot.

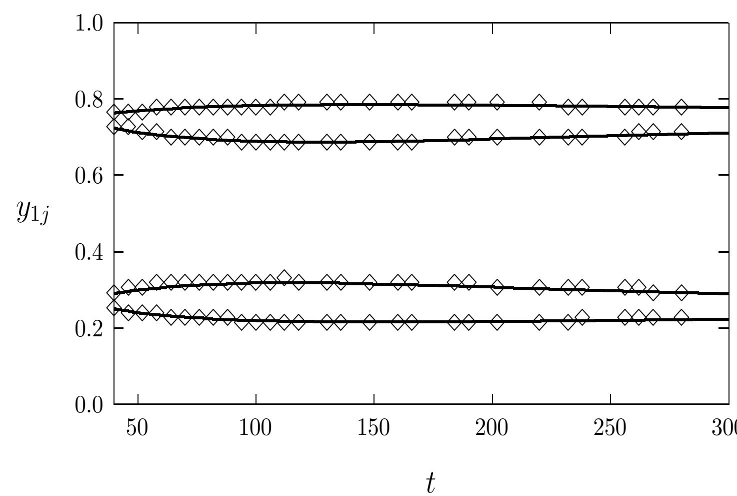
(I): $x_2(0) = (0.5, 0.8)$; $S_1 = 4.61$, $S_2 = 4.46$; Both spots split; (movie)



$t = 2.0$ $t = 33.5$ $t = 46.3$ $t = 280.3.$

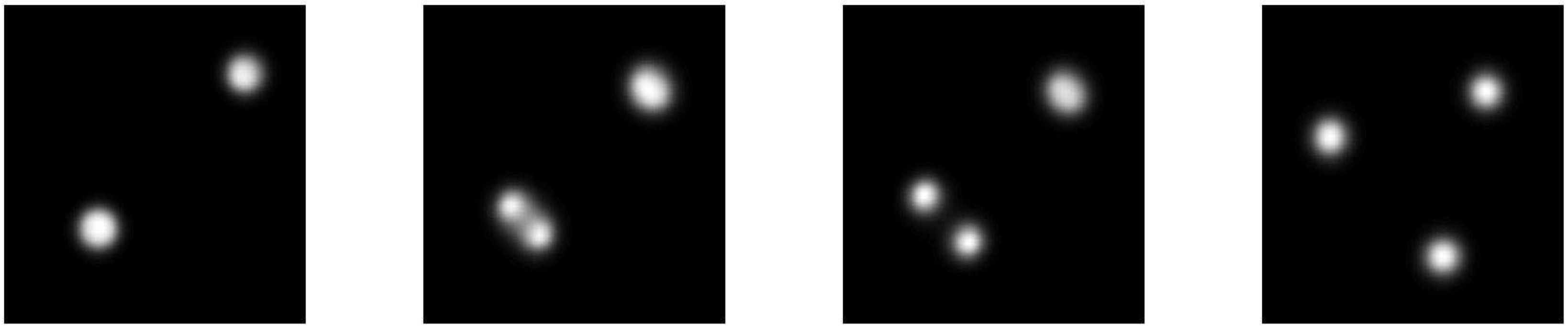
The DAE system tracks spot trajectories closely after the splitting





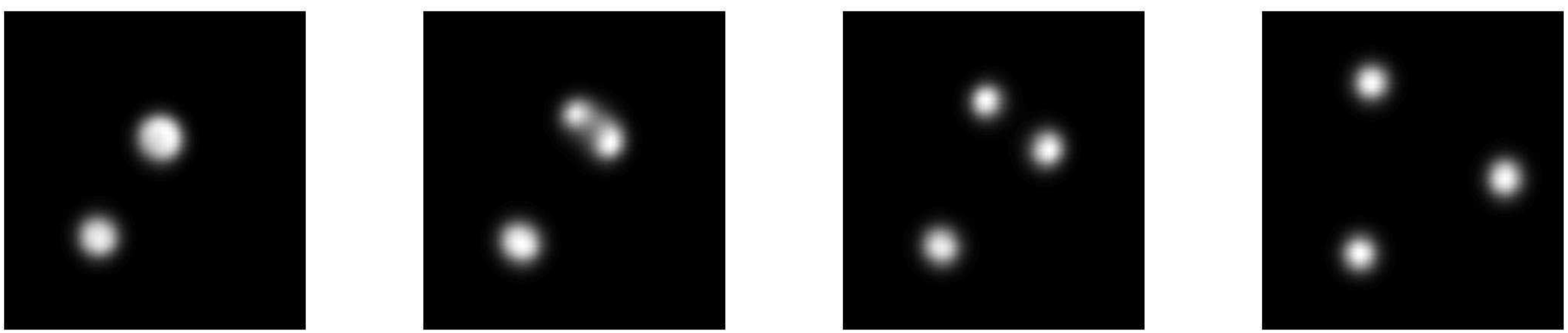
Numerical Validation, 2-Spot Solutions: II

(II): $x_2(0) = (0.8, 0.8)$; $S_1 = 5.27$, $S_2 = 3.79$; Only x_1 splits; (movie)



$t = 2.5$ $t = 19.9$ $t = 29.4$ $t = 220.3$.

(III): $x_2(0) = (0.5, 0.6)$; $S_1 = 3.67$, $S_2 = 5.39$; Only x_2 splits; (movie)



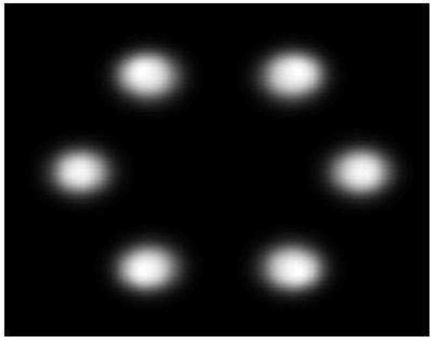
$t = 4.0$ $t = 16.5$ $t = 29.4$ $t = 322.7$.

Numerical Validation, Another Example

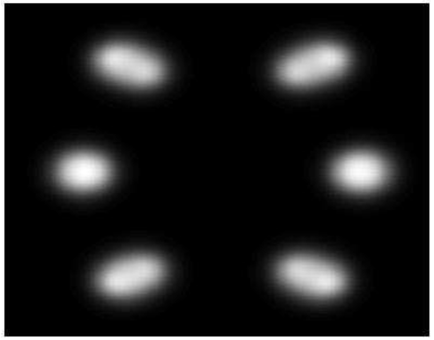
(IV): Let $\Omega = [0,1]^2$, $\varepsilon = 0.02$, $a = 51$, $D = 0.1$ and let

$$x_j = x_c + 0.33 e^{i\pi(j-1)/3}\,, \quad j = 1, \ldots, 6\,;$$

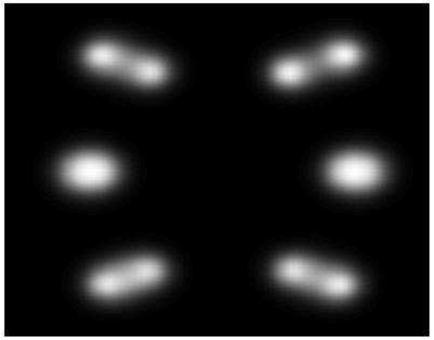
The DAE system gives $S_1 = S_4 \approx 4.01$, and $S_2 = S_3 = S_5 = S_6 \approx 4.44$. Thus, since $\Sigma_2 \approx 4.3$, we predict that four spots split (movie). The DAE system closely tracks the spots after the splitting.



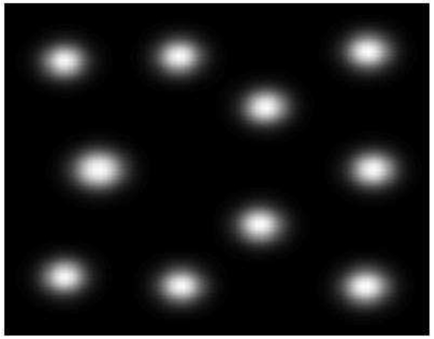
$t = 4.0$



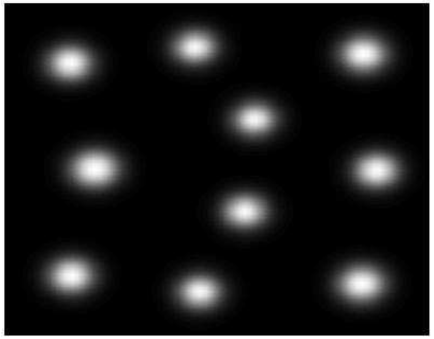
$t = 25.5$



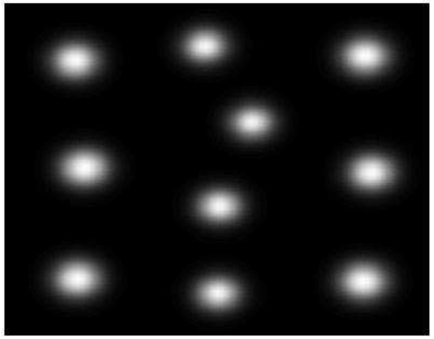
$t = 40.3.$



$t = 280.3$



$t = 460.3$



$t = 940.3.$

Ring Patterns in the Unit Disk: I

Let $\mathcal{G}$ be the (symmetric) Green's function matrix with entries $\mathcal{G}_{ii} = R$ and $\mathcal{G}_{ij} = G_{ij}$. Then:

Proposition: *Suppose that the spot locations x_j for $j = 1, \ldots, K$ are arranged so that $\mathcal{G}$ is a circulant matrix. Then, with $e = (1, \ldots, 1)^t$,*

$$\mathcal{G}e = \frac{p}{K}e \,, \qquad p = p(x_1, \ldots, x_K) \equiv \sum_{i=1}^{K}\sum_{j=1}^{K} \mathcal{G}_{ij} \,,$$

and (from the DAE system) the spots have a common source strength S_c

$$S_j \equiv S_c \equiv \frac{a|\Omega|}{2\pi K\sqrt{D}} \,, \quad j = 1, \ldots, K \,.$$

Key: For a ring pattern of spots in the unit disk, $\mathcal{G}$ is circulant. Hence, we predict the possibility of simultaneous spot-splitting events. In addition, we can derive a simple ODE for the ring radius in terms of p.

Ring Patterns in the Unit Disk: II

Analysis of the DAE system is possible for a ring pattern in the unit disk

Put K spots on a ring of radius r at the roots of unity

$$x_j = re^{2\pi ij/K}, \quad j = 1, \dots, K, \qquad \text{(Pattern I)} .$$

Then, $\mathcal{G}$ is circulant with eigenpair $e = (1, \dots, 1)^t$ and $p_K(r)/K$, where

$$p_K(r) \equiv \frac{1}{2\pi}\left[-K\log(Kr^{K-1}) - K\log\left(1 - r^{2K}\right) + r^2K^2 - \frac{3K^2}{4}\right].$$

There is a common source strength $S_c \equiv a|\Omega|/(2\pi K\sqrt{D})$. For $S_c < \Sigma_2 \approx 4.3$, the spot locations x_j satisfy the ODE's

$$x_j' \sim -\pi\varepsilon^2\gamma(S_c)S_c\frac{1}{K}p_K'(r)e^{2\pi ij/K}, \quad j = 1, \dots, K .$$

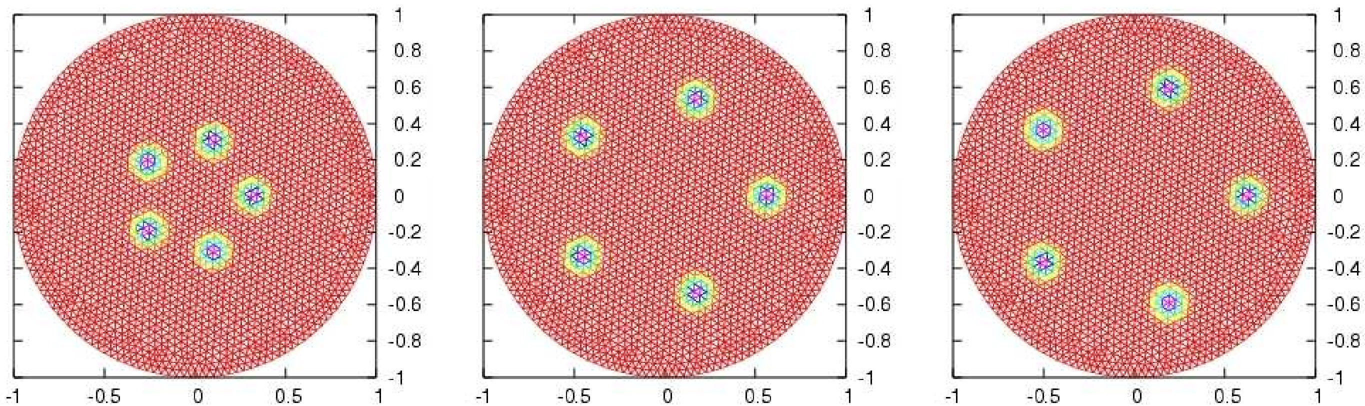
This yields an ODE for the ring radius

$$r' = -\varepsilon^2\gamma(S_c)S_c\left[-\frac{(K-1)}{2r} + \frac{Kr^{2K-1}}{1 - r^{2K}} + rK\right],$$

which has a unique stable equilibrium r_e in $0 < r_e < 1$.

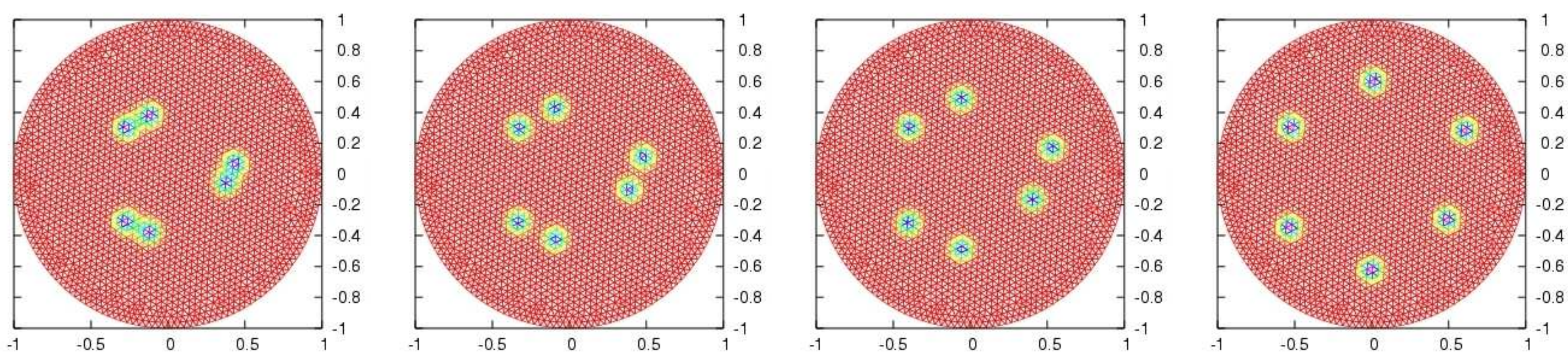
Ring Patterns in the Unit Disk: III

Experiment (Expanding Ring): $\varepsilon = 0.02$, $K = 5$, $a = 35$, and $D = 1$. Then, $S_c = 3.5 < \Sigma_2$, and the ring expands to $r_e \approx 0.625$.



$t = 8$ $t = 90$ $t = 297.$

Experiment (Spot-Splitting on a Ring): $\varepsilon = 0.02$, $K = 3$, $a = 30$, and $D = 1$. Then, $S_c = 5.0 > \Sigma_2$. Final state has 6 spots with $r_e \approx 0.642$. (movie)

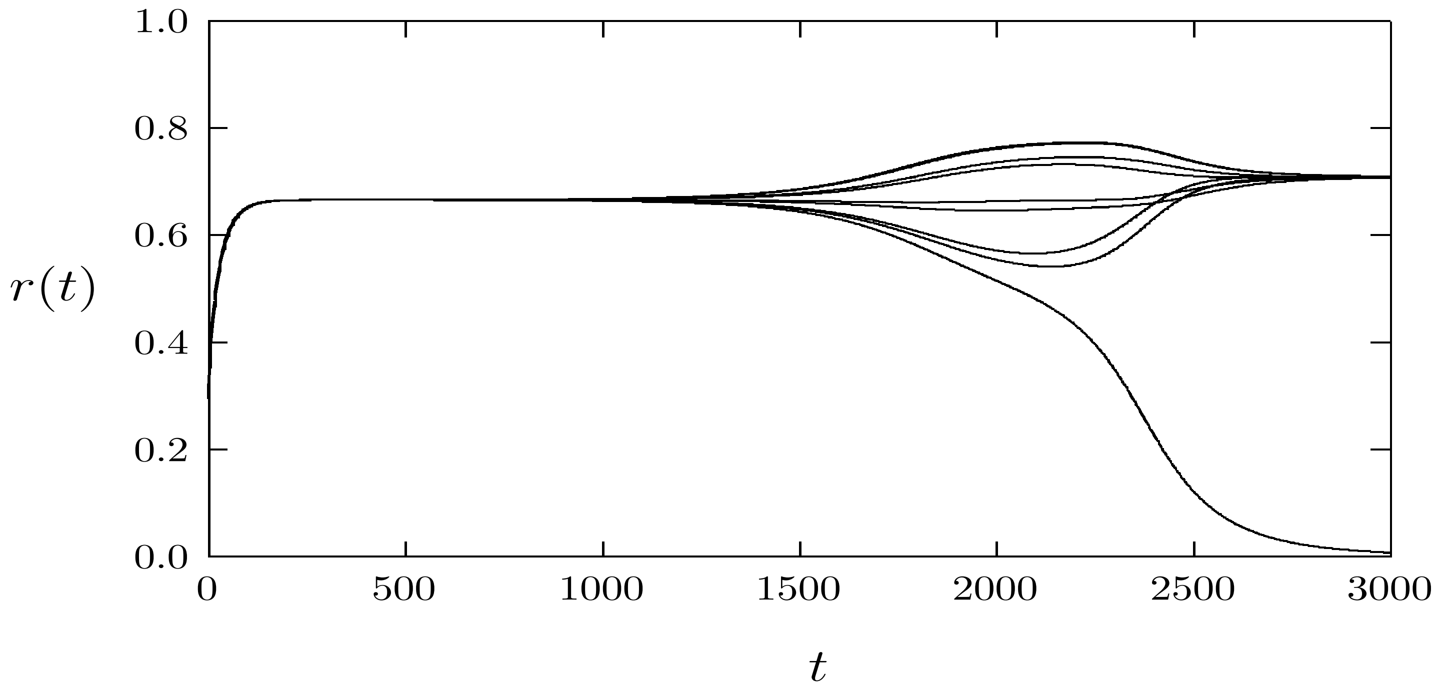


$t = 30$ $t = 45$ $t = 75$ $t = 135.$

Ring Patterns in the Unit Disk: IV

Although the radial ODE for the ring radius has a stable equilibrium, the full DAE system has a weak instability if too many spots are on one ring.

Experiment (Small Eigenvalue Instability): Choose $\varepsilon = 0.02$, $a = 60$, $K = 9$, and $D = 1$. Initially nine spots remain on a slowly expanding ring. However, the equilibrium has eight spots on a ring with a center-spot.



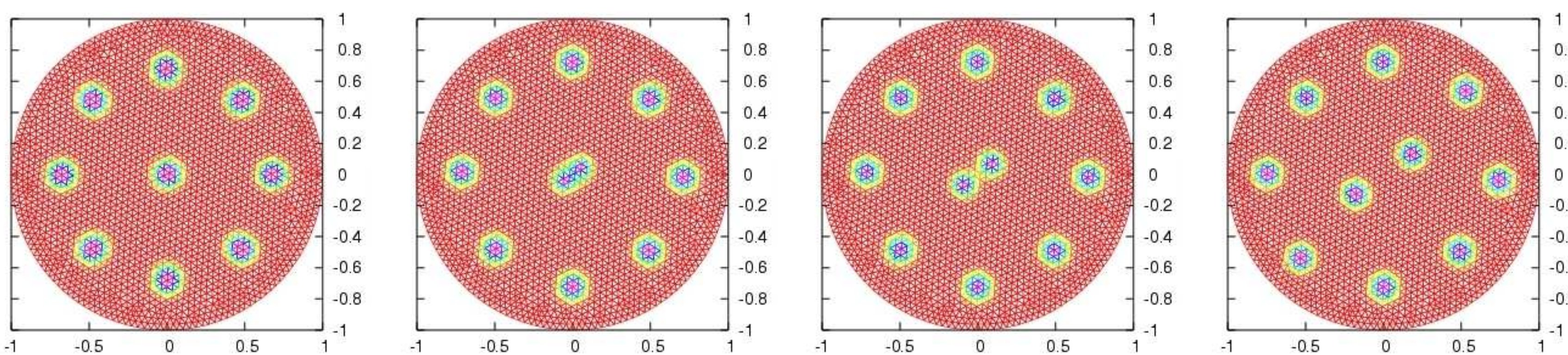
Similar weak instability to: 1) S. Gueron, I. Shafir, “On a Discrete Variational Principle Involving Interacting Particles”, SIMA, 1999. 2) Fluid vortices on the equatorial plane of a sphere (S. Boatto, Physica D 2002).

Ring Patterns in the Unit Disk: V

Consider ring pattern II consisting of spots together with a center spot of source strength S_K

Dynamic Spot-Splitting Instability: A ring pattern II that is stable at $t = 0$ can become unstable at some $t > 0$ when S_K exceeds $\Sigma_2 \approx 4.3$. Thus, as t is increased and the ring radius exceeds a critical value, a dynamic instability occurs and the center spot splits before the equilibrium ring radius is achieved.

Experiment: $\varepsilon = 0.02$, $K = 9$, $a = 74$, and $D = 1$. The center-spot eventually splits since $S_K > \Sigma_2$ at some $t = T$ with $T > 0$. (movie).



$t = 54$ $t = 372$ $t = 387$ $t = 800$.

GS Model: Brief Overview of 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 types of instabilities of spots: self-replication, oscillatory instability, annihilation or overcrowding Instability.
- Calculate a phase diagram classification for various symmetric arrangements of spots.
- Ph.D thesis work of Wan Chen, UBC.

GS Model: Dynamics of Spots

Collective Slow Coordinates: S_j and x_j, for $j = 1, \ldots K$.

Principal Result: (DAE System): *Let* $\mathcal{A} = \varepsilon A/(\nu\sqrt{D})$ *and* $\nu = -1/\log\varepsilon$. *The DAE system for 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* $R(x_j; x_j)$, *i.e.*

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

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

GS Model: Three Types of Spot Instabilities

- **M=2 Mode:** The core problem is asymptotically the same as for Schakenburg. Hence, J^{th} spot splits iff $S_J > \Sigma_2 \approx 4.3$.
- **M=0 Mode:** Stability problem is formulated as:

$$\mathcal{L}_0 \Phi_j - \Phi_j + 2U_j V_j \Phi_j + V_j^2 N_j = \lambda \Phi_j \,,$$

$$\mathcal{L}_0 N_j - V_j^2 N_j - 2U_j V_j \Phi_j = 0 \,,$$

$$\Phi_j \to 0 \,, \quad N_j \to C_j \left(\log \rho + B_j \right) \,, \quad \rho \to \infty \,,$$

These inner problems are coupled through the outer problem as

$$C_j (1 + 2\pi\nu R_{\lambda\, jj}) + \nu B_j + \sum_{i=1, i\neq j}^{K} \nu\, C_i G_{\lambda ij} = 0 \,, \quad \text{for } j = 1, \ldots, K \,.$$

The G-function $G_\lambda(x; x_j)$ with regular part $R_\lambda(x; x_j)$ satisfy

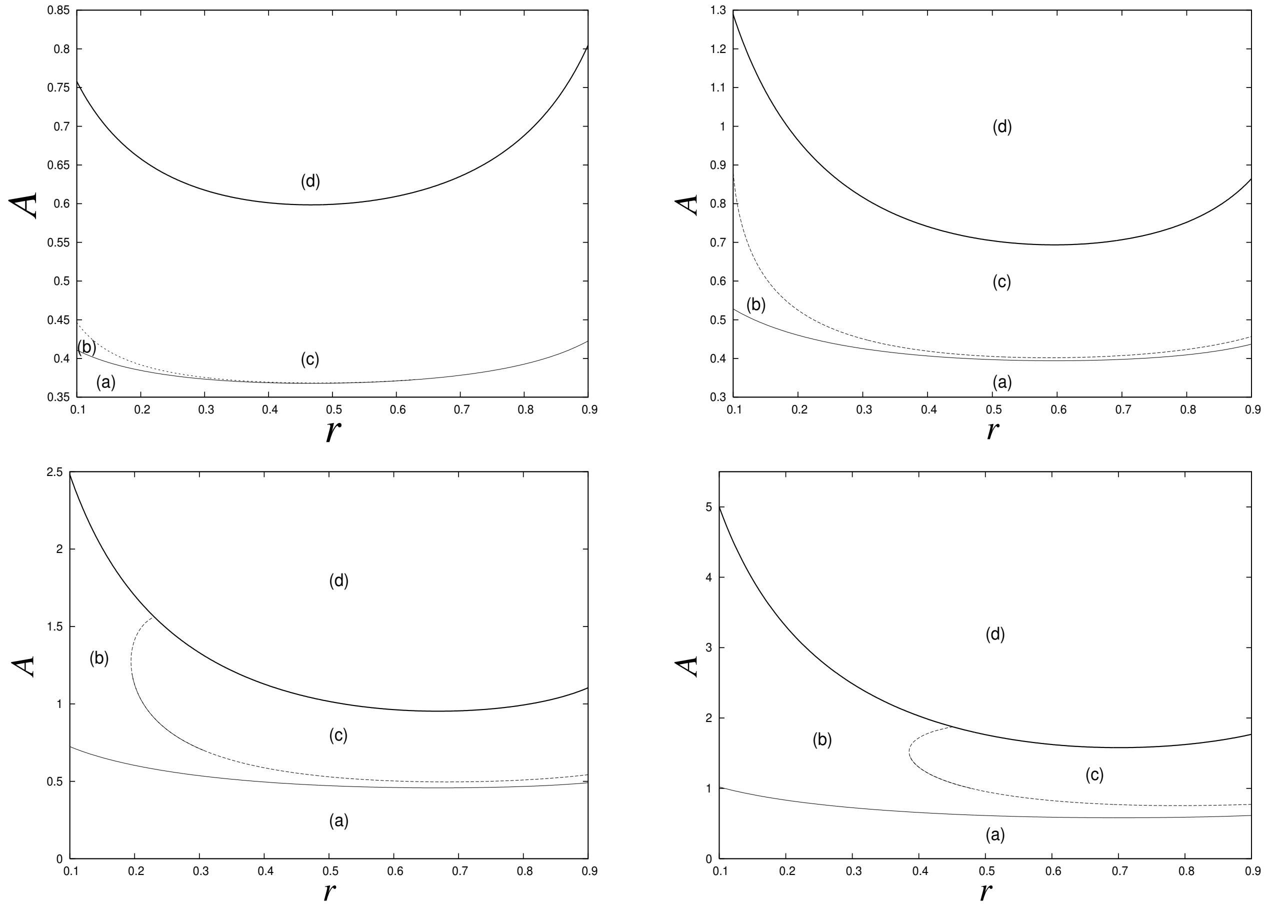
$$\Delta G_\lambda - \frac{(1+\tau\lambda)}{D} G_\lambda = \delta(x - x_j) \,, \quad \partial_n G_\lambda = 0 \,, \quad x \in \partial\Omega \,,$$

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

To leading order in ν we can get an NLEP problem. Numerical Computations: Annihilation or Oscillatory Instabilty.

Phase Diagram: Spots on a Ring in Unit Disk

- Phase diagram $\mathcal{A}$ versus r for $K = 2, 4, 8, 16$ spots on a ring of radius r with $D = 0.2$.
- **Regions:** (a) Non-existence; (b) Annihilation instability; (c) Oscillatory instability with large τ; (d) Spot-replication.



Open Issues and Further Directions

- **Green's Function (PDE):** Rigorous results needed for critical points of regular part of Neumann and Reduced-wave Green's functions.
- **Rigour:** existence and stability theory for coupled core problem. Rigorous derivation of DAE system for spot dynamics?
- **Universality:** Apply framework to RD systems with classes of kinetics, to derive general principles for dynamics, stability, replication.
- **Other Related Models:** self-replication in integro-differential models of Fisher type (B. Perthame ..)?
- **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).
- **Patterns on Growing Domains and on Manifolds:** Delayed bifurcation effects, and require Green's functions on manifolds.
- **Fractional Diffusion:** Theory largely based on large diffusivity ratio. Can one do a similar theory when the activator has subdiffusive fractional diffusion (due to binding/unbinding events on crowded substrate) while the inhibitor diffuses freely? (inspired by talk of A. Marciniak-Czopra in Brazil, March 2009).

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Available at: http://www.math.ubc.ca/ ward/prepr.html

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Lecture II:

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