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

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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

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

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.

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).
  \[ g(u, v) = -v + v^p / u^q, \quad f(u, v) = -u + v^r / u^s. \]

- **GS Model**: (Pearson, 1993, Swinney 1994, Nishiura et al. 1999)
  \[ g(u, v) = -v + Auv^2, \quad f(u, v) = (1 - u) - uv^2. \]

- **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.

Self-Replicating Spot Behavior: I

Experimental evidence of spot-splitting


Self-Replicating Spot Behavior: II

Numerical evidence of spot-splitting


Right: Muratov and Osipov (1996).
Self-Replicating Spot Behavior: IV

Numerical evidence of spot-splitting


**Schnakenburg Model:**
Self-Replicating Spots for Schnakenburg

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.
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, Promisloow, 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 $\varepsilon$.
- 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 $\Omega$, with $\varepsilon \ll 1$ is

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

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

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

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

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 $D \gg 1$, $\nabla R_{d0}$ can be approximated by $\nabla R_0$, 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 $R_h$:

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

$$H(x, x_0) = -\frac{1}{2\pi} \log|x - x_0| + R_h(x; x_0), \quad \nabla R_{h_0} \equiv \nabla R_h(x, x_0)|_{x=x_0}.$$

For a strictly convex domain $\Omega$, $R_{h_0}$ is strictly convex, and thus there is a unique root to $\nabla R_{h_0} = 0$. (B. Gustafsson, Duke J. Math (1990), Caffarelli and Friedman, Duke Math J. (1985)).

$\nabla R_{h_0}$ can be found for certain mappings $f(z)$ of the unit disk as

$$f'(z_0)\nabla R_{h_0} = -\frac{1}{2\pi} \left( \frac{z_0}{1 - |z_0|^2} + \frac{f''(\overline{z_0})}{2f'(\overline{z_0})} \right).$$

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 $\nabla R_{h_0} = 0$ 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 \( \lambda_1 \) of the Laplacian with one localized trap of radius \( \varepsilon \)

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

Thus, \( \lambda_1 \) is maximized for a symmetric dumbbell-shaped domain by putting the trap at the center of the neck (which is intuitively clear).
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 $\nu$ 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 $\Omega$ consider

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

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


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).

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 \( V(y) \) and \( U(y) \) by

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

To leading order, \( U \sim U(\rho) \) and \( V \sim V(\rho) \) (radially symmetric) with \( \rho = |y| \).
This yields the coupled core problem with \( U'(0) = V'(0) = 0 \), where:

\[
  V_{\rho\rho} + \frac{1}{\rho} V_{\rho} - V + UV^2 = 0, \quad U_{\rho\rho} + \frac{1}{\rho} U_{\rho} - UV^2 = 0, \quad 0 < \rho < \infty,
\]

\[
  V \to 0, \quad U \sim S \log \rho + \chi(S) + o(1), \quad \text{as} \quad \rho \to \infty.
\]

- 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 \( \varepsilon^{-2}uv^2 \to 2\pi\sqrt{D}S\delta(x - x_0) \). 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

\[
u(x) = -\frac{2\pi}{\sqrt{D}}(SG(x; x_0) + u_c),
\]

where \( S + 2\pi\nu SR(x_0; x_0) + \nu\chi(S) = -2\pi\nu u_c, \quad \nu \equiv -1/\log \varepsilon.\)
The Quasi-Equilibrium Solution: IV

Remarks On Asymptotic Construction:

- $G$, its regular part $R$, and their gradients, can be calculated for different $\Omega$. (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 $O(1)$ 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

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

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

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

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

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

$\bullet$ $U$ and $V$ are computed from the core problem and depend on $S$.

$\bullet$ **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 \( \Sigma_m \) being the value of \( S \) such that \( \text{Re} \lambda_0(\Sigma_m, m) = 0 \).

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

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

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

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

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

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 $\nu$, 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 $D = 0(\nu^{-1}) \gg 1$:** 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

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

- **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 $\lambda_0(S, 2) \approx 0.15$. 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 vary $x_2(0)$, the initial location of the second spot.

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

The DAE system tracks spot trajectories closely after the splitting.
Numerical Validation, 2-Spot Solutions: II

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

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

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

$t = 4.0$
$t = 16.5$
$t = 29.4$
$t = 322.7$
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.
Let $G$ be the (symmetric) Green’s function matrix with entries $G_{ii} = R$ and $G_{ij} = G_{ji}$. Then:

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

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

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, $G$ 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 $p$. 
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

$$x_j = re^{2\pi ij/K}, \quad j = 1, \ldots, K,$$

(Pattern I).

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

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

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

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

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 $r_e \approx 0.625$.

![Images of ring patterns at different times](image1)

$t = 8$

$t = 90$

$t = 297$

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)

![Images of spot patterns at different times](image2)

$t = 30$

$t = 45$

$t = 75$

$t = 135$. 
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.

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).
GS Model: Brief Overview of Case Study

GS Model: in a 2-D domain $\Omega$ consider the GS model

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

- 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 \( A = \varepsilon A/(\nu \sqrt{D}) \) and \( \nu = -1/\log \varepsilon \). The DAE system for the source strengths \( S_j \) and spot locations \( x_j \) is

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

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

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, \( J^{\text{th}} \) spot splits iff \( S_J > \Sigma_2 \approx 4.3 \).

**M=0 Mode:** Stability problem is formulated as:

\[
\begin{align*}
\mathcal{L}_0 \Phi_j - \Phi_j + 2U_j V_j \Phi_j + V_j^2 N_j &= \lambda \Phi_j , \\
\mathcal{L}_0 N_j - V_j^2 N_j - 2U_j V_j \Phi_j &= 0 , \\
\Phi_j &\to 0 , \quad N_j &\to C_j (\log \rho + B_j) , \quad \rho &\to \infty ,
\end{align*}
\]

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

\[
\begin{align*}
\Delta G_\lambda - \frac{(1 + \tau \lambda)}{D} G_\lambda &= \delta(x - x_j) , \quad \partial_n G_\lambda = 0 , \quad x \in \partial \Omega , \\
G_\lambda(x; x_j) &\sim \frac{1}{2\pi} \log |x - x_j| + R_\lambda(x; x_j) , \quad \text{as } x \to x_j .
\end{align*}
\]

To leading order in \( \nu \) we can get an NLEP problem. Numerical Computations: Annihilation or Oscillatory Instability.
Phase Diagram: Spots on a Ring in Unit Disk

- Phase diagram $A$ 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 $\tau$; (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).
References I

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

Lecture I:


Lecture II:


