Topics in Localized Pattern Formation in 3-D

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Shanghai Workshop: Emerging Areas in Reaction-Diffusion Systems

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Outline: Emerging Areas for RD Modeling

**Topic I:** Localized Spot Patterns for RD systems in 3-D domains (Schnakenburg model). Quasi-equilibria, stability, slow dynamics, and effect of heterogeneities (Tzou, Xie, Kolokonikov)

**Topic II:** Berg-Purcell Problem Revisited. Determination of effective capacitance of a sphere with $N$ small “traps” on the boundary. The homogenized limit and the mean first capture time. (Lindsay, Bernoff)

**Topic III:** Analysis of coupled bulk-surface RD systems. Weakly nonlinear theory for patterns near onset (F. Paquin-Lefebvre (PhD thesis work), Nagata).

Some Novel Features:

- Derivation and study of new discrete variational problems (Topics I, II).
- The novel effect of coupling of PDEs of different “dimensions” leads to a new type of linear stability problem with Steklov structure (Topic III).
In dimensionless form, the Schnakenberg RD model for $\Omega \in \mathbb{R}^3$ is:

$$
\begin{align*}
\mathcal{V}_t &= \varepsilon^2 \Delta \mathcal{V} + b - \mathcal{V} + \mathcal{U} \mathcal{V}^2, \quad x \in \Omega; \quad \partial_n \mathcal{V} = 0, \quad x \in \partial \Omega, \\
\mathcal{U}_t &= \mathcal{D} \Delta \mathcal{U} + A - \mathcal{U} \mathcal{V}^2, \quad x \in \Omega, \quad \partial_n \mathcal{U} = 0, \quad x \in \partial \Omega.
\end{align*}
$$

Here, $\mathcal{V}$ and $\mathcal{U}$ are the activator and inhibitor, while $A$ is the feed-rate. Localized spot solutions occur in the regime $\mathcal{D} = \mathcal{O}(\varepsilon^{-4})$. We introduce

$$
\mathcal{U} = \varepsilon^3 u, \quad \mathcal{V} = \varepsilon^{-3} v, \quad \mathcal{D} = \varepsilon^{-4} D,
$$

and discard the negligible $\varepsilon^3 b$ term. This yields:

$$
\begin{align*}
\mathcal{V}_t &= \varepsilon^2 \Delta \mathcal{V} - \mathcal{V} + \mathcal{V}^2, \quad x \in \Omega; \quad \partial_n \mathcal{V} = 0, \quad x \in \partial \Omega, \\
\varepsilon^3 \mathcal{U}_t &= \frac{D}{\varepsilon} \Delta \mathcal{U} + A - \frac{\mathcal{U} \mathcal{V}^2}{\varepsilon^3}, \quad x \in \Omega; \quad \partial_n \mathcal{U} = 0, \quad x \in \partial \Omega.
\end{align*}
$$

A localized spot pattern is where $\mathcal{V}$ concentrates as $\varepsilon \to 0$ at a discrete set of points $x_1, \ldots, x_N$ in $\Omega$.

Slowly Increasing the Feed in a Sphere

Self-replication events when slowly increasing the feed rate $A$ for $\varepsilon = 0.03$, $D = 1$, and $A$ is slowly increased from 1 to 400 according to $A = 1 + 0.0036t$. Left: snapshots of solution for several values of $A$. Right: the number of spots as a function of $A$: full FLEXPDE6 numerics compared with leading-order asymptotics $A_{N,max} \sim 253.33N\sqrt{D/|\Omega|}$. [Movie]
Coarsening when slowly decreasing the feed rate $A$ for $\varepsilon = 0.03$, $D = 1$, and $A$ is decreased from 400 to 1 by $A = 400 - 0.0036t$. Left: snapshots of solution for several values of $A$. Right: the number of spots as a function of $A$: full FLEXPDE6 numerics compared with leading-order asymptotics $A_{N,\text{min}} \sim 56.8N \sqrt{D}/|\Omega|$. ([Movie])
The Spot Profile: Core Problem

“Freeze” the spot locations $x_j$, for $j = 1, \ldots, N$. In the $j$-th inner region:

$$v = \sqrt{D} [V_{j0}(\rho) + O(\varepsilon)] , \quad u = \frac{1}{\sqrt{D}} [U_{j0}(\rho) + O(\varepsilon)] , \quad y = \varepsilon^{-1}(x - x_j) ,$$

and $\rho = |y|$. This yields the BVP core problem on $0 < \rho < \infty$:

$$\Delta_\rho V_{j0} - V_{j0} + U_{j0}V_{j0}^2 = 0 , \quad V_{j0} \to 0 , \quad \text{as} \quad \rho \to \infty ,$$

$$\Delta_\rho U_{j0} - U_{j0}V_{j0}^2 = 0 , \quad U_{j0} \sim \mu_0 - S_j / \rho , \quad \text{as} \quad \rho \to \infty ,$$

where $\Delta_\rho V_{j0} \equiv V_{j0}'' + 2\rho^{-1}V_{j0}'$ and $\mu_0 = \mu_0(S_j)$ is to be computed.

Left: $\mu_0 = \mu_0(S_j)$ with minimum at $(S_{cf}, \mu_{0f}) \approx (4.52, 5.78)$. Right: $V_{j0}(\rho)$ for $S_j = 4$ (dotted), $S_j = 18$ (dashed), and $S_j = 29$ (solid). Note: $U_{j0} \not\to 0$ as $\rho \to \infty$. 
Quasi-Equilibria: Collection of Spots

Asymptotic matching of $N$ core solutions to an outer (inhibitor) field gives

$$u = \xi - \frac{4\pi \varepsilon}{\sqrt{D}} \sum_{i=1}^{N} S_{i\varepsilon} G(x; x_i), \quad \sum_{i=1}^{N} S_{i\varepsilon} = \frac{A|\Omega|}{4\pi \sqrt{D}},$$

where $G(x; \xi)$ is the Neumann Green’s function

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

$$G(x; \xi) = \frac{1}{4\pi|x - \xi|} + R(x; \xi), \quad \text{as} \quad x \to \xi; \quad \int_{\Omega} G \ dx = 0.$$

Comparing the singularity behavior gives a weakly coupled nonlinear algebraic system (NAS) for $\xi, S_{1\varepsilon}, \ldots, S_{N\varepsilon}$ in terms of $\mu_0(S_{j\varepsilon})$ and $G$:

$$\xi - \frac{4\pi \varepsilon}{\sqrt{D}} (G S)_{j} = \frac{\mu_0(S_{j\varepsilon})}{\sqrt{D}}, \quad j = 1, \ldots, N; \quad \sum_{j=1}^{N} S_{j\varepsilon} = \frac{A|\Omega|}{4\pi \sqrt{D}}.$$

Here $S \equiv (S_{1\varepsilon}, \ldots, S_{N\varepsilon})^T$, and $G$ is the symmetric Neumann Green’s matrix with entries $(G)_{ij} = G(x_j; x_i)$ for $i \neq j$ and $(G)_{jj} = R_j \equiv R(x_j; x_j).$
Quasi-Equilibria: Role of $\mathcal{G}$: I

Imperfection sensitivity occurs for spot configurations for which $e = (1, \ldots, 1)^T$ is not an eigenvector of $\mathcal{G}$. Illustrate with $N = 2$ spots.

![Graph](https://via.placeholder.com/150)

Caption: $\sqrt{\frac{1}{N} \sum S_j^2}$ versus $A|\Omega|/(4\pi N \sqrt{D})$ for $D = 0.1$ and $\varepsilon = 0.05$.

Left: antipodal spots at $x_1 = (0, 0, r_0)$ and $x_2 = -x_1$ with $r_0 = 0.429$ in unit sphere: $\mathcal{G}e = \kappa_1 e$. Transcritical bifurcation observed.

Right: spots at $x_1 = (0, 0, r_0 + 0.1)$ and $x_2 = (0, 0, -r_0)$: $\mathcal{G}e \neq k_1 e$. Imperfection sensitivity occurs. Dashed curves: $S_1 < S_{cf} < S_2$ or $S_2 < S_{cf} < S_1$. Solid curves: either $S_1, S_2 > S_{cf}$ or $S_1, S_2 < S_{cf}$.
Quasi-Equilibria: Role of $G$: II

For $N = 2$, suppose $R_1 \neq R_2$, i.e. $Ge \neq \kappa_1 e$: (two non-antipodal spots)

$$S_1 + S_2 = \frac{A|\Omega|}{4\pi \sqrt{D}}, \quad \mu_0(S_1) - \mu_0(S_2) = -4\pi \varepsilon [R_1 S_1 - R_2 S_2 + (S_2 - S_1)G_{12}].$$

A local “unfolding” analysis near $S_{cf}$ gives a parameterization

$$\frac{A|\Omega|}{4\pi (2) \sqrt{D}} \sim S_{cf} + \left( \frac{\delta_{0d}}{2} \right) x\varepsilon^{2/3}, \quad S_{1,2} \sim S_{cf} \pm \varepsilon^{1/3} S_{0d} y + \left( \frac{\delta_{0d}}{2} \right) x\varepsilon^{2/3},$$

in terms of roots $(x, y)$ of the canonical cubic

$$y^3 - xy = 1.$$

Here $S_{0d}$ and $\delta_{0d}$ are defined by

$$S_{0d} = \left( \frac{12\pi S_{cf} (R_1 - R_2)}{|\mu_0'''(S_{cf})|} \right)^{1/3}, \quad \delta_{0d} = \left( \frac{|\mu_0'''(S_{cf})|}{3} \right)^{1/3} \left[ \frac{4\pi S_{cf} (R_1 - R_2)}{\mu_0''(S_{cf})} \right]^{2/3}.$$

Conclusion: fold point for manifold of 2-spot quasi-equilibria is at

$$\left( \frac{A|\Omega|}{4\pi (2) \sqrt{D}} \right)_{\text{fold}} \sim S_{cf} + \left( \frac{\delta_{0d}}{2} \right) x_{\text{min}} \varepsilon^{2/3}, \quad S_{cf} \approx 4.52, \quad x_{\text{min}} \approx 1.8899.$$
Quasi-Equilibria: Imperfect Bifurcation

Caption: Comparison with asymptotic result (light solid curve) obtained from cubic with $\varepsilon = 0.05$ and $D = 1$.

Conjecture: As the feed-rate $A$ is decreased an $N$-spot quasi-equilibrium pattern undergoes a coarsening process (annihilation of spots) by falling off of a slow manifold of quasi-equilibria at a fold point.

For $N$-spot quasi-equilibria and for $|S_c - S_{cf}| \gg \mathcal{O}(\varepsilon^{1/3})$, a two-term expansion for $\varepsilon \ll 1$ for the solution branch with $S_j = \mathcal{O}(1)$ $\forall j$ and

$$S_j \varepsilon \sim S_c + \frac{4\pi \varepsilon S_c}{\mu_0(S_c)} \left( \frac{e^T G e}{N} - (G e)_j \right) + \cdots , \quad j = 1, \ldots, N .$$
Spot Annihilation: Competition Instability

Let $v_{qe}$ and $u_{qe}$ be the quasi-equilibrium pattern with frozen $x_1, \ldots, x_N$:

$$v = v_{qe} + e^{\lambda t} \phi, \quad u = u_{qe} + e^{\lambda t} \psi,$$

(Linearization).

For $|x - x_j| = \mathcal{O}(\varepsilon)$, we look for locally radially symmetric perturbations:

$$\phi \sim c_j \Phi_j(\rho), \quad \psi \sim c_j \Psi_j(\rho)/D.$$

We match to an outer solution, and use $S_j \sim S_c \forall j$. In terms of the canonical inner problem,

$$\Delta_\rho \Phi_c - \Phi_c + 2V_c U_c \Phi_c + V_c^2 \Psi_c = \lambda \Phi_c, \quad \Phi_c \to 0, \quad \text{as } \rho \to \infty,$$

$$\Delta_\rho \Psi_c - 2V_c U_c \Phi_c - V_c^2 \Psi_c = 0, \quad \Psi_c \sim \frac{1}{\rho} + B(\lambda; S_c), \quad \text{as } \rho \to \infty,$$

for $N \geq 2$, we derive to leading-order that the discrete eigenvalues $\lambda$ for instabilities of locally radially symmetric perturbations are roots of

$$B(\lambda; S_c) = 0.$$

The allowable amplitude perturbations $c = (c_1, \ldots, c_N)^T$ is the $N - 1$ dimensional subspace where $e^T c = 0$ and $e^T = (1, \ldots, 1)$. 
The real (left) and imaginary (right) parts of the eigenvalue with largest real part satisfying $B(\lambda; S_c) = 0$. As $S_c$ decreases, there is a complex conjugate pair of eigenvalues that collide on the negative real axis when $S_c \approx 5.12$. As $S_c$ is decreased further, a real eigenvalue crosses into the right half-plane when $S_c = S_{cf} \approx 4.52$. Further numerics shows that $B(i\lambda, S_c) \neq 0$.

**Key Observation:** Differentiating the core problem with respect to $S_c$, we conclude that $B(0; S_{cf}) = 0$, where $\mu'_0(S_{cf}) = 0$. Thus, a zero-eigenvalue crossing occurs at the minimum of the graph of $\mu_0$ versus $S_c$. 
Left: Surface plot of $v$ on the plane $z = 0$ for two antipodal spots initially at $(0, \pm 0.429, 0)$. Right: amplitudes of the two spots for $D = 0.143$, $\varepsilon = 0.01$, and $A = 10$ so that $S_c \approx 4.4 < S_{\text{comp}}$. The linear competition instability is seen to trigger a nonlinear event leading to the collapse of one of the two spots.

Leading-order theory: competition stability threshold is independent of the spatial configuration $x_1, \ldots, x_N$. This is qualitatively different than in 2-D. Can we calculate the $O(\varepsilon)$ correction to the thresholds?
Main Result: Let $\varepsilon \to 0$ and $N \geq 2$, and suppose that $G\mathbf{e} = k_1\mathbf{e}$, with $\mathbf{e} = (1, \ldots, 1)^T$. Then, an $N$-spot quasi-equilibrium solution is linearly stable to a competition instability on an $O(1)$ time-scale iff

$$S_c > S_{\text{comp}, \varepsilon} \equiv S_{cf} - \frac{4\pi \varepsilon}{\mu''_0(S_{cf})} \min_{j=2, \ldots, N} \kappa_j,$$

where

$$S_c \equiv \frac{A|\Omega|}{4\pi N \sqrt{D}},$$

and $S_{cf} \approx 4.52$. Here $\kappa_j$ are eigenvalues in the orthogonal subspace $G\mathbf{c}_j = \kappa_j \mathbf{c}_j$ with $\mathbf{c}_j^T \mathbf{e} = 0$ for $j = 2, \ldots, N$. Equivalently, no instabilities iff

$$D < D_{\text{comp}} \equiv \frac{(A|\Omega|)^2}{16\pi^2 N^2} \left( S_{cf} - \frac{4\pi \varepsilon}{\mu''_0(S_{cf})} \min_{j=2, \ldots, N} \kappa_j \right)^{-2},$$

$$A > A_{\varepsilon} \equiv A_{N, \text{min}} \left[ 1 - \frac{4\pi \varepsilon}{S_{cf} \mu''_0(S_{cf})} \min_{j=2, \ldots, N} \kappa_j \right],$$

where $A_{N, \text{min}} \equiv 4\pi N \sqrt{D} S_{cf} / |\Omega| \approx 56.8 N \sqrt{D} / |\Omega|$.

Verify this for the unit sphere, where $G$ can be found explicitly using

$$G(\mathbf{x}; \xi) = \frac{1}{4\pi |\mathbf{x} - \xi|} + \frac{1}{4\pi |\mathbf{x}| |\mathbf{x}' - \xi|} + \frac{1}{4\pi} \log \left( \frac{2}{1 - \mathbf{x} \cdot \xi + |\mathbf{x}| |\mathbf{x}' - \xi|} \right) + \frac{1}{8\pi} \left( |\mathbf{x}|^2 + |\xi|^2 \right) - \frac{7}{10\pi}.$$
Refined competition stability threshold (solid curves) compared with FLEXPDE6 results for two antipodal spots at $x_1 = (0, 0, r_0)$ and $x_2 = -x_1$ for $A = 10$ and $\varepsilon = 0.03$ inside the unit ball. The solid (open) dots correspond to where the pattern was observed numerically from FLEXPDE6 to be stable (unstable). The horizontal dotted lines are the leading-order competition thresholds $D_{\text{comp}} \approx 0.136$ (left) and $S_{\text{comp}} \equiv S_{cf} \approx 4.52$ (right).
Spot Self-Replication I

Shape-Deforming Instability of a localized spot determined by spectrum of non-radially symmetric solutions tending to zero of local problem:

\[ \Delta_y \Phi - \Phi + 2U_c V_c \Phi + V_c^2 \Psi = \lambda \Phi, \quad \Delta_y \Psi - 2U_c V_c \Phi - V_c^2 \Psi = 0. \]

Here \( U_c \) and \( V_c \) satisfy the core problem with source strength \( S \). Setting

\[ \Phi = P_\ell^m(\cos \phi)e^{im\theta} F(\rho), \quad \Psi = P_\ell^m(\cos \phi)e^{im\theta} H(\rho), \]

where \( y^t = \rho(\sin \phi \cos \theta, \sin \phi \sin \theta, \cos \phi) \), with \( 0 < \phi < \pi \) and \( 0 < \theta \leq 2\pi \).

We obtain the local eigenvalue problem on \( 0 < \rho < \infty \):

\[ \mathcal{L}_\ell F - F + 2U_c V_c F + V_c^2 H = \lambda F, \quad F(0) = 0, \quad F \to 0, \quad \text{as} \quad \rho \to \infty, \]

\[ \mathcal{L}_\ell H - 2U_c V_c F - V_c^2 H = 0, \quad H(0) = 0, \quad H \sim \frac{1}{\rho^{\ell+1}}, \quad \text{as} \quad \rho \to \infty, \]

where \( \mathcal{L}_\ell \equiv \partial_{\rho\rho} + 2\rho^{-1} \partial_{\rho} - \ell(\ell + 1)\rho^{-2} \).

Numerically compute for each \( l = 1, 2, \ldots \), \( \lambda_{\text{max}} \) versus \( S \) and look for zero-eigenvalue crossings.
Spot Self-Replication II

Caption: $\Re \lambda_{max}$ versus $S$ for $\ell = 2$ (heavy solid), $\ell = 3$ (light solid), and $\ell = 4$ (dashed). As $S$ increases, the $\ell = 2$ mode is the first to become unstable.

**Leading-order theory:** $N$-spot quasi-equilibria are linearly stable on an $O(1)$ time-scale to shape-deformation iff

$$S_j \sim S_c \equiv \frac{A|\Omega|}{4\pi N \sqrt{D}} < \Sigma_2 \approx 20.16.$$ 

- **FLEXPDE6:** suggests that such linear instabilities are subcritical and trigger spot self-replication.
- Since to leading order $S_j \sim S_c \forall j$, we predict simultaneous spot-splitting as $A$ increases independent of $x_1, \ldots, x_N$. (Not quite)
Spot Self-Replication III

Refined Theory: Since

\[ S_j \varepsilon \sim S_c + \frac{4\pi \varepsilon S_c}{\mu'_0(S_c)} \left( \frac{e^T \mathbf{Ge}}{N} - (\mathbf{Ge})_j \right), \quad j = 1, \ldots, N, \]

the largest \( S_j \) corresponds to \( \min_{j=1,\ldots,N} (\mathbf{Ge})_j \). Thus, as \( A \) is increased past \( A_{c,\varepsilon} \), the spot that splits should be the one with the smallest value of \( (\mathbf{Ge})_j \). Here, with \( A_{N,\text{max}} \equiv 4\pi N \Sigma_2 \sqrt{D/|\Omega|} \approx 253.3 N \sqrt{D/|\Omega|}, \)

\[ A_{c,\varepsilon} = A_{N,\text{max}} \left[ 1 + \frac{4\pi \varepsilon}{\mu'_0(S_c)} \left( \frac{e^T \mathbf{Ge}}{N} - \min_{j=1,\ldots,N} (\mathbf{Ge})_j \right) \right]. \quad \text{(Movie)} \]
**Slow Spot Dynamics I**

**Main Result:** When the $N$-spot quasi-equilibrium is linearly stable to both competition and peanut-splitting instabilities, the ODE-DAE system

$$\frac{dx_j}{dt} = \frac{12\pi \varepsilon^3}{\kappa_1} \left( S_j \varepsilon \nabla_x R(x; x_j)|_{x=x_j} + \sum_{i \neq j}^N S_i \varepsilon \nabla_x G(x; x_i)|_{x=x_j} \right), \quad j = 1, \ldots, N,$$

characterizes the slow spot dynamics. Here $S_1 \varepsilon, \ldots, S_N \varepsilon$ satisfy the NAS

$$\xi - \frac{4\pi \varepsilon}{\sqrt{D}} (GS)_j = \frac{\mu_0(S_j \varepsilon)}{\sqrt{D}}, \quad j = 1, \ldots, N; \quad \sum_{j=1}^N S_j \varepsilon = \frac{A|\Omega|}{4\pi \sqrt{D}},$$

where $\kappa_1 = \kappa_1(S_j \varepsilon) < 0$. To leading-order, $S_j \sim S_c \equiv A|\Omega|/(4\pi N \sqrt{D})$, which yields the gradient flow dynamics

$$\frac{dx_j}{dt} = -\frac{6\pi \varepsilon^3 S_c}{|\kappa_1|} \nabla_{x_j} \mathcal{H}(x_1, \ldots, x_N); \quad \mathcal{H} \equiv \sum_{i=1}^N R(x_i; x_i) + \sum_{i=1}^N \sum_{j \neq i}^N G(x_i; x_j).$$

**Key:** If $x_1, \ldots, x_N$ is a local minimum of $\mathcal{H}$ it is a linearly stable equilibrium of the gradient flow. But, as $N$ increases, the energy landscape of $\mathcal{H}$ has many local minima. Basin of attraction of equilibria for spot dynamics?
Left: $\kappa_1$ versus $S_c$. Note: $\kappa_1 < 0$ for $0 < S_c < \Sigma_2 \approx 20.16$.

Right: $z_0(t)$ coordinate of two antipodal spots initially located at $(0, 0, \pm 0.1375)$. FLEXPDE6 (solid) and ODE (circles). Parameters: $D = 1$, $A = 80$, and $\varepsilon = 0.02$.

**Example (Unit Sphere):** For two antipodal spots $x_1 = (0, 0, z_0)$ and $x_2 = -x_1$,

$$\frac{dz_0}{dt} = -\frac{A\varepsilon^3}{2\sqrt{D}|\kappa_1|} F_2(z_0), \quad F_2(z_0) \equiv \frac{2z_0^3(3 - z_0^4)}{(z_0^4 - 1)^2} + 2z_0 - \frac{1}{4z_0^2},$$

$\exists$ a unique root $z_{0e}$ to $F_2(z_0) = 0$ on $0 < z_0 < 1$ given by $z_{0e} \approx 0.42885$. 
Spot Equilibria and the MFPT

Relation to MFPT: For $\varepsilon \to 0$, the configuration $x_1, \ldots, x_N$ that globally minimizes $\mathcal{H}$ is the configuration of the centers of $N$ small spherical traps that globally minimizes the averaged MFPT $\bar{T}$ for

$$\Delta T = -\frac{1}{D}, \quad x \in \Omega \setminus \Omega_a \equiv \bigcup_{j=1}^{N} \Omega_{\varepsilon,j} ; \quad \partial_n T = 0, \quad x \in \partial \Omega,$$

$$T = 0, \quad x \in \partial \Omega_{\varepsilon,j}, \quad j = 1, \ldots, N.$$ 

Here $\Omega_{\varepsilon,j}$ is a sphere of radius $\varepsilon$ centered at $x_j \in \Omega$. From [CW], as $\varepsilon \to 0$

$$\bar{T} \equiv \frac{1}{|\Omega \setminus \Omega_a|} \int_{\Omega \setminus \Omega_a} T \, dx \sim \frac{|\Omega|}{4\pi \varepsilon ND} \left[ 1 + \frac{4\pi \varepsilon}{N} \mathcal{H}(x_1, \ldots, x_N) \right],$$

Ref: [CW], Cheviakov, MJW, Optimizing the Fundamental Eigenvalue... Math. Comp. Mod. 53, (2011).
## Equilibria of Spot Dynamics: Unit Sphere

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<th>$\mathcal{H}_0^{(b)}$</th>
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**Caption:** In unit sphere, optimize $\mathcal{H}$ restricted to either ring or ring+center pattern. Define $\mathcal{H}_0$ by $\mathcal{H} = \frac{\mathcal{H}_0}{4\pi} - \frac{7N^2}{10\pi}$.

- **N=12:** Some initial conditions lead to a steady-state with spots at vertices of an icosahedron. Others lead to a ring+center pattern.
- **N=13,...,20:** (Restricted) global min of $\mathcal{H}$ correspond (closely) to stable spot equilibria with large basins of attraction.
- **N=5:** For random IC, the gradient flow tends to a steady-state with 2 antipodal spots and 3 spots equally-spaced on a mid-plane.
Spot Dynamics: Heterogeneous Feed I

What is the effect of a spatially heterogenous feed-rate $A(x)$?

Suppose that the feed-rate models a localized source of fuel, i.e.

$$A(x) = A_0 + B\delta(x - \xi),$$

where $A_0 > 0$, $B > 0$, and $\xi \in \Omega$. For a one-spot solution the source-strength $S_1$ depends on $\bar{A} = A_0 + B/|\Omega|$.

The slow one-spot dynamics in the unit sphere, with $r = |x_1|$, satisfies

$$\frac{dx_1}{dt} = -\frac{3\varepsilon^3 S_1}{|\kappa_1|} \left[ x_1 \left( \frac{(2 - r^2)}{(1 - r^2)^2} + 1 \right) - \frac{3B}{A_0 + B/|\Omega|} \nabla_x G(x; \xi)|_{x=x_1} \right],$$

with $S_1 = \bar{A}/(3\sqrt{D})$, and where $\nabla_x G(x; \xi)|_{x=x_1}$ is obtained explicitly.

Spot Pinning: If $x_1(0)$ is sufficiently close to the fuel source $\xi$, the ODE dynamics yields $x_1(T) = \xi$ at some $t = T < \infty$.

New Equilibrium: If $x_1(0)$ is not close to $\xi$, and $B$ not too large, the spot reaches a new steady-state determined by a competition between the localized fuel and the center of the sphere.
Spot Dynamics: Heterogeneous Feed II

Left: ODE spot dynamics in unit sphere versus FLEXPDE6 (dotted) for $D = 1$ and $\varepsilon = 0.03$ with localized feed $A(x) = A_0 + B\delta(x - \xi)$. Here $A_0 = 20$, $B = 20|\Omega|$, with $|\Omega| = 4\pi/3$, and $\xi = (0, 0, 0.5)$. We plot $|x_1(t) - \xi|$ versus $t$ for three initial conditions: $x_1(0) = (0, 0.7, -0.2)^T$ (heavy solid), $x_1(0) = (-0.7, -0.2, -0.6)^T$ (solid), and $x_1 = (-0.5, 0.0, 0.0)^T$ (dotted). Right: boundaries for domain of attraction for 3 ratios $B/A_0$.

Self-Replication-Annihilation Attractor for the Schnakenburg model in 2-D with a localized but moving fuel source. (Movie) (with Tony Wong; ongoing)
**$D = \mathcal{O}(\varepsilon)$: Spots to/from Tubes**

Our analysis of spots has focused on the regime $D = \mathcal{O}(1)$ for

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

$$\varepsilon^3 u_t = \frac{D}{\varepsilon} \Delta u + A - \frac{uv^2}{\varepsilon^3}, \quad x \in \Omega; \quad \partial_n u = 0, \quad x \in \partial\Omega.$$

Key Question: What patterns occur if $D/\varepsilon = \mathcal{O}(1)$?

For $D = \mathcal{O}(\varepsilon)$, for which is $D/\varepsilon = D_0 = \mathcal{O}(1)$, there appears to be no quasi-equilibrium spot pattern. Problem: the leading-order outer problem $\mathcal{D}_0 \Delta u + A = \sum_j (\ldots) \delta(x - x_j)$ cannot satisfy $u \sim \mu_0(S_j)(\ldots)$ as $x \to x_j$, since $\mu_0(S_j) > 0$.

- $\varepsilon = 0.03, \ D/\varepsilon = 1/20$. Clustered Spots to Tubes are observed as $A$ increases. **(Movie)** As $A$ increases slowly in time above $A \approx 350$ there appears to be a transition to the tubed state.

- $\varepsilon = 0.03, \ D/\varepsilon = 1/20$. Tubes to Clustered Spots are observed as $A$ decreases. **(Movie)**
Caption: spherical target centered at $x_0 \in \Omega$ of radius $\varepsilon \ll 1$, with $N$ locally circular absorbing surface nanotrap of radii $\sigma \ll \varepsilon$ modeled by homogeneous Dirichlet condition.

- The Brownian particle diffuses in $\Omega$ until captured by one of the $N$ small absorbing traps on the boundary of the target sphere. How long (on average) does it take to get captured?

- The small spherical target has radius $\varepsilon \ll 1$. The disk-shaped surface traps have a common radius $\sigma$ with $\sigma \ll \varepsilon$ and are centered at $x_j$ for $j = 1, \ldots, N$. 
The Narrow Capture Time PDE

The Mean First Passage Time (MFPT) $T$ satisfies

$$\Delta T = -\frac{1}{D}, \quad x \in \Omega \setminus \Omega_{\varepsilon}; \quad \partial_n T = 0, \quad x \in \partial \Omega,$$

$$T = 0, \quad x \in \partial \Omega_{\varepsilon a} ; \quad \partial_n T = 0, \quad x \in \partial \Omega_{\varepsilon r},$$

where $\partial \Omega_{\varepsilon a}$ and $\partial \Omega_{\varepsilon r}$ are the absorbing and reflecting part of the surface.

- Calculate the averaged MFPT $\bar{T}$ for capture of a Brownian particle.
- $\bar{T}$ depends on the capacitance $C_0$ of the structured target (related to the Berg-Purcell problem, 1977).
- Derive new discrete optimization problems characterizing the optimal MFPT and determine how the fragmentation of the trap set affects $\bar{T}$.

Ref: [LBW2017] Lindsay, Bernoff, MJW, First Passage Statistics for the Capture of a Brownian Particle by a Structured Spherical Target with Multiple Surface Traps, SIAM Multiscale Mod. and Sim. 15(1), (2017), pp. 74–109.
Receptor Binding and Narrow Capture II

Using strong localized perturbation theory, for $\varepsilon \to 0$ the average MFPT is

$$\bar{T} \equiv \frac{1}{|\Omega \setminus \Omega_\varepsilon|} \int_{\Omega \setminus \Omega_\varepsilon} T d\mathbf{x} = \frac{|\Omega|}{4\pi C_0 D\varepsilon} \left[ 1 + 4\pi \varepsilon C_0 R(x_0) + O(\varepsilon^2) \right],$$

where $R(x_0)$ is the regular part of the Neumann Green’s function for $\Omega$.

Capacitance Problem: “exterior” problem in potential theory. $C_0$ satisfies

$$\Delta v = 0, \quad \mathbf{y} \in \mathbb{R}^3 \setminus \Omega_0; \quad v = 0, \quad \mathbf{y} \in \Gamma_a, \quad \partial_n v = 0, \quad \mathbf{y} \in \Gamma_r,$$

$$\lim_{R \to \infty} \int_{\partial \Omega_R} \partial_n v \, ds = -4\pi; \quad v \sim -\frac{1}{C_0} + \frac{1}{|\mathbf{y}|} + O(|\mathbf{y}|^{-2}), \quad |\mathbf{y}| \to \infty.$$

Main Result: For $\sigma \to 0$, [LBW2017] derived that

$$\frac{1}{C_0} = \frac{\pi}{N\sigma} \left[ 1 + \frac{\sigma}{\pi} \left( \log \left( 2e^{-3/2}\sigma \right) + \frac{4}{N} \mathcal{H}(\mathbf{y}_1, \ldots, \mathbf{y}_N) \right) + O(\sigma^2 \log \sigma) \right].$$

Calculating $C_0$: Berg-Purcell Problem I

Left: Nanotraps at vertices of dodecahedron. Right: 1001 Nanotraps at vertices of Spiral Fibonacci points.

The discrete energy $\mathcal{H}(y_1, \ldots, y_N)$, with constraint $|y_j| = 1 \ \forall j$, is

$$\mathcal{H}(y_1, \ldots, y_N) \equiv \sum_{j=1}^{N} \sum_{k=j+1}^{N} g(|y_j - y_k|); \quad g(\mu) \equiv \frac{1}{\mu} + \frac{1}{2} \log \mu - \frac{1}{2} \log(2 + \mu).$$

Here $g(|y_j - y_k|) = 2\pi G_s(y_j; y_k)$, $G_s$ is the surface-Neumann G-function

$$G_s(y_j; y_k) = \frac{1}{2\pi} \left[ \frac{1}{|y_j - y_k|} - \frac{1}{2} \log \left( \frac{1 - y_j \cdot y_k + |y_j - y_k|}{|y_j| - y_j \cdot y_k} \right) \right].$$
Calculating $C_0$: Berg-Purcell Problem II

Remarks:

- On $0 < \mu < 2$, the particle-particle interaction energy $g(\mu)$ is monotone decreasing, positive, and convex.

- The minimization of $\mathcal{H}$, which will maximize $C_0$, is a new variational problem of Fekete-point type.

Key Steps in Derivation

- Asymptotic expansion of global (outer) solution and local (inner) solutions near each trap (using tangential-normal coordinates).

- The surface G-function has a subdominant logarithmic singularity on the boundary (related to surface diffusion). This fact requires adding “logarithmic switchback terms in $\varepsilon$” in the outer expansion.

- The leading-order local solution is the tangent plane approximation and yields electrified disk problem in a half-space, with capacitance $c_j$.

Key: Need corrections to the tangent plane approximation in the inner region near the trap. This higher order term in the inner expansion satisfies a Poisson-type problem, with monopole far-field behavior.

- Asymptotic matching and solvability conditions yield $1/C_0$. 
Calculating $C_0$: Berg-Purcell Problem III

Formal Large $N$ Limit: For $N$ large and “uniformly distributed points”, for which we expect $C_0$ to be “maximized”, we have

$$\mathcal{H} \sim \frac{N^2}{4} - d_1 N^{3/2} + \frac{1}{8} N \log N + d_2 N + d_3 N^{1/2} + \cdots .$$

With $d_1 = 1/2$, $d_2 = 1/8$ and $d_3 = 1/4$. Better to use $d_1 = 0.55230$ for “pure” Coulombic interactions [Saff]. This gives a new scaling law:

Main Result: For $N \gg 1$, but small trap surface area fraction $f = \mathcal{O}(\sigma^2 \log \sigma)$ and uniformly distributed points, we have:

$$\frac{1}{C_0} \sim 1 + \frac{\pi \sigma}{4f} \left( 1 - \frac{8d_1}{\pi} \sqrt{f} + \frac{\sigma}{\pi} \log \left( \beta \sqrt{f} \right) + \frac{2d_3 \sigma^2}{\pi \sqrt{f}} \right), \quad \beta \equiv 4e^{-3/2} e^{4d_2}. $$

Homogenized Robin Condition: This yields the effective trapping rate $\kappa_h$:

$$\Delta v_h = 0, \quad |y| > 1; \quad \partial_n v_h + \kappa v_h = 0, \quad |y| = 1; \quad v_h(y) \sim \frac{1}{|y|}, \quad |y| \to \infty,$$

$$\kappa_h \sim \frac{4f}{\pi \sigma} \left[ 1 - \frac{8d_1}{\pi} \sqrt{f} + \frac{\sigma}{\pi} \log \left( \beta \sqrt{f} \right) + \frac{2d_3 \sigma^2}{\pi \sqrt{f}} \right]^{-1}. $$
Calculating $C_0$: Berg-Purcell Problem IV

Berg-Purcell Result: is the leading-order term $\frac{1}{C_0} \sim 1 + \frac{\pi \sigma}{4f}$. Our analysis provides correction terms for the sphere. Most notable is $\sqrt{f}$ term.

Numerics: Compare scaling law with full numerics from fast multipole theory based on integral equations [Bernoff, Lindsay]

Effect of Fragmentation: fix trap area fraction $f$, increase $N$, and choose “optimal” points. Recall: $f = \frac{N\pi \sigma^2}{[4\pi]}$.

![Graph](image)

Caption: From top to bottom: $f = \{0.02, 0.05, 0.1, 0.15\}$ For $N = 2000$, $f = 0.02$, numerics gives $C_0^{-1} = 1.1985$ and $C_0^{-1} = 1.2028$ (scaling law).

Conclusion: Fragmentation effects are significant until $N$ becomes large.
Clustering and Fragmenting the Trap Set

Caption: $N = 20$ identical and equally spaced nanotraps (centers shown only) clustered in the polar region $\theta \in (0, \frac{\pi}{3})$ with total absorbing fraction $f = 0.05$. Blue trap: is the equivalent area as a single nanotrap. Radius of nanotraps is $\sigma = 2 \sqrt{f/N}$.

$$\frac{1}{C_0} \approx 5.41 \text{ (Single Trap)}; \quad \frac{1}{C_0} \approx 2.79 \text{ (clustered)}; \quad \frac{1}{C_0} \approx 1.98 \text{ (optimal)}.$$

**Conclude I:** subdividing a single nanotrap into 20 smaller, but clustered, nanotraps of same total area roughly halves the MFPT to the target.

**Conclude II:** The MFPT for 20 optimally distributed traps is significantly smaller than for 20 clustered traps.
**Topic III: Bulk-Surface RD Systems**

**Bulk-Surface RD Model:** coupling passive diffusion in a bulk domain with a reaction-diffusion process on the domain boundary. Coupling is done through Robin boundary conditions between bulk and surface.


- Finite elements, rigorous theory (Elliot, Madzvamuse, Roger,...)

**Our Focus:** For a class of coupled bulk-surface RD model in a disk, develop a weakly nonlinear theory for pattern formation near bifurcation points. Derive and analyze amplitude equations for Hopf, Turing, Turing-Hopf instabilities. **Thesis work of Paquin-Lefebvre (UBC)**
Coupled Membrane-Bulk System I

Dimensionless Formulation: Let \( \Omega = \{ \mathbf{x} \in \mathbb{R}^2 \mid \| \mathbf{x} \| < R \} \). In the bulk, we assume passive diffusion

\[
\frac{\partial U}{\partial t} = D_u \Delta U - \sigma_u U, \quad \frac{\partial V}{\partial t} = D_v \Delta V - \sigma_v V, \quad \mathbf{x} \in \Omega, \quad t > 0,
\]
coupled to the surface with the Robin boundary condition

\[
D_u \frac{\partial U}{\partial r} \bigg|_{r=R} = K_u (u - U|_{r=R}), \quad D_v \frac{\partial V}{\partial r} \bigg|_{r=R} = K_v (v - V|_{r=R}).
\]

This 2-D bulk problem is coupled to a nonlinear 1-D RD system on the boundary (membrane) of the circular disk

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \frac{d_u}{R^2} \frac{\partial^2 u}{\partial \theta^2} - K_u (u - U|_{r=R}) + f(u, v), \\
\frac{\partial v}{\partial t} &= \frac{d_v}{R^2} \frac{\partial^2 v}{\partial \theta^2} - K_v (v - V|_{r=R}) + g(u, v).
\end{align*}
\]

Coupled Membrane-Bulk System II

Outline of Analysis:

- Construct radially symmetric steady-state solution \( u_e(r) \), and linearize introducing \( u = u_e + e^{\lambda t + in\theta} \Phi \). Derive the eigenvalue relation. Linearization is not around a spatially uniform state.

- Plot marginal stability curves for Hopf \( n = 0 \) and Turing \( n = 1 \) branches. The bifurcation parameters are taken as \( D_v \) and \( K_v \), and we consider any such two-parameter path crossing a marginal stability boundary.

- Key step: formulate appropriate adjoint of linearized operator, inner product, orthogonality relation, and solvability condition.

- Multi-scale expansion in order to derive normal form amplitude equations for Hopf, Turing, and Turing-Hopf instabilities. Central is to derive explicit “computable” formulae for the coefficients for arbitrary \( f \) and \( g \).
Membrane-Bulk: WNA (Technical I)

\[ \dot{W} = \mathbf{F}(W) = \begin{pmatrix} D_u \Delta U - \sigma_u U \\ D_v \Delta V - \sigma_v V \\ \frac{d_u}{R^2} u_{\theta \theta} - K_u (u - U) + f(u, v) \\ \frac{d_v}{R^2} v_{\theta \theta} - K_v (v - V) + g(u, v) \end{pmatrix} \]

for functions satisfying

\[ W \in \mathcal{W} \equiv \left\{ \begin{pmatrix} U(r, \theta) \\ V(r, \theta) \\ u(\theta) \\ v(\theta) \end{pmatrix} \middle| D_u \partial_r U|_{r=R} = K_u (u - U|_{r=R}) \right. \]

For a radially symm. base-state \( W_e(r) \in \mathcal{W} \), let \( \tilde{W} = W - W_e \). Expand

\[ \dot{\tilde{W}} = \mathcal{L}\tilde{W} + \mathcal{B}(\tilde{W}, \tilde{W}) + \mathcal{C}(\tilde{W}, \tilde{W}, \tilde{W}) + \ldots , \]

where \( \mathcal{L}\tilde{W} \) is the linearized operator with eigenfunctions \( \mathcal{L}\Phi_n = \lambda \Phi_n \),

\[ \mathcal{L}(\tilde{W}) = \begin{pmatrix} D_u \Delta \tilde{U} - \sigma_u \tilde{U} \\ D_v \Delta \tilde{V} - \sigma_v \tilde{V} \\ \frac{d_u}{R^2} \tilde{u}_{\theta \theta} - K_u \left( \tilde{u} - \tilde{U} \right) + f_u^e \tilde{u} + f_v^e \tilde{v} \\ \frac{d_v}{R^2} \tilde{v}_{\theta \theta} - K_v \left( \tilde{v} - \tilde{V} \right) + g_u^e \tilde{u} + g_v^e \tilde{v} \end{pmatrix} , \quad \text{where} \quad \Phi_n = \begin{pmatrix} \tilde{W}_1(r)e_1^T \phi_n \\ \tilde{W}_2(r)e_2^T \phi_n \\ \phi_n \end{pmatrix} e^{i n \theta} \].
**Membrane-Bulk: WNA (Technical II)**

**Stability Threshold:** \( \text{Re}(\lambda_{\text{max}}(n, \mu_0)) = 0 \) for \( n = 0, 1, 2, \ldots \) and \( \mu_0 \equiv (K_v, D_v)^T \). Derive the adjoint \( \mathcal{L}^*(W^*) \) and introduce inner product

\[
\langle W^*, W \rangle = \int_0^{2\pi} \int_0^R \left[ U^* U + V^* V \right] r dr d\theta + \int_{\partial \Omega} \left[ u^* u + v^* v \right] d\sigma ,
\]

where \( W \equiv (U, V, u, v)^T \) and \( W^* \equiv (U^*, V^*, u^*, v^*)^T \).

**Fredholm Alternative Lemma:** Let \( \lambda_c \) denote the critical eigenvalue at a given bifurcation point \( \mu_0 = (K_c^v, D_c^v) \). Then,

\[
\mathcal{L}(\mu_0; \Phi_n) = \lambda_c \Phi_n , \quad \mathcal{L}^*(\mu_0; \Phi_n^*) = \overline{\lambda_c} \Phi_n^* , \quad \lambda_c \equiv \begin{cases} i \lambda & n = 0 \\ 0 & n \neq 0 \end{cases} .
\]

Consider the inhomogeneous problem

\[
\lambda_c X - \mathcal{L}(\mu_0; X) = \mathcal{F} \quad \text{with} \quad \left[ \partial_r \left( \frac{D_u x_1}{D_v x_2} \right) \bigg|_{r=R} - \left( \frac{K_u (x_3 - x_1|_{r=R})}{K_v (x_4 - x_2|_{r=R})} \right) \right] = \begin{pmatrix} \xi(\theta) \\ \eta(\theta) \end{pmatrix} ,
\]

where \( X \equiv (x_1(r, \theta), x_2(r, \theta), x_3(\theta), x_4(\theta))^T \). A necessary condition for a solution is

\[
\langle \Phi_n^*, \mathcal{F} \rangle + \int_{\partial \Omega} \overline{U_n^*} \xi \ d\sigma + \int_{\partial \Omega} \overline{V_n^*} \eta \ d\sigma = 0 .
\]
Membrane-Bulk: Normal Forms

Two-parameter sweep across linear stability boundary \((K_v^c, D_v^c)^T\):

\[
\mu = (K_v^c, D_v^c)^T + \varepsilon^2 \mu_1.
\]

The weakly nonlinear theory (WNA) yields Normal Forms:

\[
\frac{dA_0}{d\tau} = g^T_{1000} \mu_1 A_0 + g_{2100} |A_0|^2 A_0, \quad \text{(Hopf)},
\]

\[
\frac{dA_n}{d\tau} = g^T_{0010} \mu_1 A_n + g_{0021} |A_n|^2 A_n, \quad \text{(Pitchfork)}.
\]

and the codimension-two Turing-Hopf:

\[
\frac{dA_0}{d\tau} = g^T_{1000} \mu_1 A_0 + g_{2100} |A_0|^2 A_0 + g_{1011} |A_n|^2 A_0,
\]

\[
\frac{dA_n}{d\tau} = g^T_{0010} \mu_1 A_n + g_{0021} |A_n|^2 A_n + g_{1110} |A_0|^2 A_n.
\]

WNA provides explicit formulae for all the coefficients in the normal form.

**Example**: Consider Brusselator membrane kinetics

\[
f(u, v) = a - (b+1)u + u^2 v, \quad g(u, v) = bu - u^2 v; \quad a > 0, \quad 0 < b < a^2 + 1.
\]
Caption: Linear stability phase diagram in \((K_v, D_v)\) plane with \(R = 1, D_u = 1, \sigma_u = \sigma_v = 0.01, K_u = 0.1, d_u = d_v = 0.5, a = 3\) and \(b = 7.5\) (left) and \(b = 8.7\) (right). Right: "o" indicates supercritical and "+" indicates subcritical.

Caption: Transition from a super to sub-critical Hopf bifurcation. Plot of the normal form coefficient \(\text{Re}(g_{2100})\) along Hopf stability curve for \(b = 8.7\).
Membrane-Bulk: Supercritical Hopf

Caption: Supercritical Hopf: $b = 7.5$ and $K_v = 5$. Left: global periodic solution branches (AUTO). Right: local branching: weakly nonlinear vs. AUTO

Caption: Left: parameter path $\mu = (K_v, D_v) = (5, 2.32)^T + \varepsilon^2 (0, 1)^T$, $\varepsilon = 0.1$. Right: weakly nonlinear vs. full numerics for membrane oscillations.
**Membrane-Bulk: Subcritical Hopf**

Caption: Subcritical Hopf: $b = 8.7$ and $D_v = 9$. Left: global periodic solution branches (AUTO). Right: local branching: weakly nonlinear vs. AUTO

Caption: Left: parameter path with $D_v = 9$ and $\varepsilon = 0.1$. Middle: $U(r, t)$ for bulk. Right: relaxation oscillations for membrane oscillations.
Membrane-Bulk: Subcritical Pitchfork

Left: parameter path with $D_v = 5$, $b = 7.5$, and $\varepsilon = 0.075$. Right: WNA approx (solid), stable branches by time-stepping to steady state in full numerics.

Stable membrane pattern at $t = 1000$ (red curve) as evolved from the unstable branch near a subcritical pitchfork.
Membrane-Bulk: Supercritical Pitchfork

Same parameters except now \( b = 5 \) and \( d_u = d_v = 1.0 \). Pitchfork is now supercritical.

Left: bifurcation diagram (AUTO) versus WNA. Right: stable Turing pattern.
Final Remarks: (My) Emerging Frontiers

- Localized patterns for RD systems in 3-D.
- Membrane-bulk coupled RD systems (modeling, stability theory, localized patterns, bifurcation software).
- Discrete variational problems and interacting particle systems arising from asymptotic reductions of RD systems.
- Creation-annihilation “chaotic” attractors.
- PDE/ODE Models of quorum and diffusion sensing: Collective oscillations in “cells” driven by intercellular chemical signalling.