

Moving Boundary Problems on Moving Cell Boundaries

Asymptotic limits of models for receptor-ligand interactions on moving domains

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a talk based on joint work with

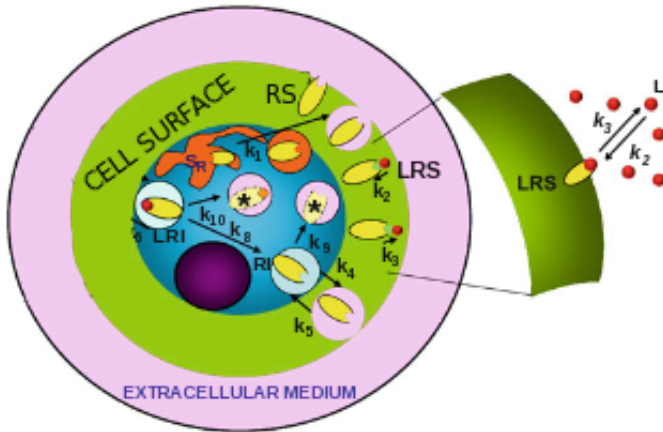
A. Alphonse (WIAS), D. Caetano and C. Elliott (Warwick)

The 81st Fujihara Seminar
Mathematical Aspects for Interfaces and Free Boundaries



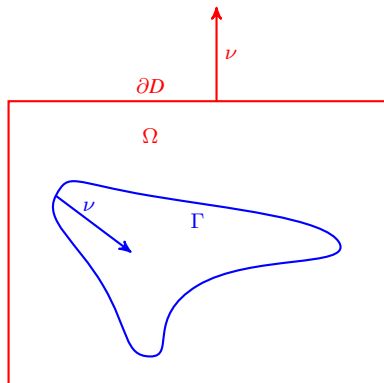
Receptor-ligand dynamics

- Primary mechanism by which cells sense and respond to their environment.
- Important in cell biological phenomena such as proliferation, motility, the maintenance of structure or form, adhesion, cellular signalling, etc.



(García-Peñarrubia, Gálvez, and Gálvez, 2013)

Coupled bulk-surface model for receptor-ligand dynamics (Elliott, Ranner, and Venkataraman, 2017)



- u : Bulk ligand concentration
- w : Surface receptor density
- z : Surface receptor-ligand complex density

Model

$$\delta_{\Omega} \partial_t u - \Delta u = 0 \quad \text{in } \Omega$$

$$u = u_D \text{ or } \nabla u \cdot \nu = 0 \quad \text{on } \partial D$$

$$\nabla u \cdot \nu = \frac{1}{\delta_{k'}} z - \frac{1}{\delta_k} u w \quad \text{on } \Gamma$$

$$\partial_t w - \delta_{\Gamma} \Delta_{\Gamma} w = \frac{1}{\delta_{k'}} z - \frac{1}{\delta_k} u w \quad \text{on } \Gamma$$

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Asymptotic limits

- Biologically relevant scales:

$$0 < 1/\delta_{k'} \ll 1$$

- We set $1/\delta_{k'} = 0$ and hence neglected z .
- Existence and uniqueness.
- Convergence to limiting free boundary problems for the cases
 - 1 $\delta_k \rightarrow 0$
 - 2 $\delta_k = \delta_{\Gamma} \rightarrow 0$
 - 3 $\delta_k = \delta_{\Gamma} = \delta_{\Omega} \rightarrow 0$
- Formulation of the limits as Stefan-type surface FBP.
- Uniqueness for the limiting FBP (2 and 3).
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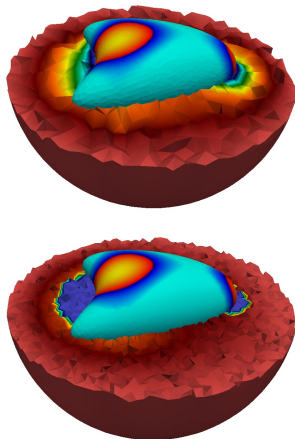
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The asymptotic limits ($\delta_k \rightarrow 0$) lead to interesting FBP's due to the complementarity nature of the resulting limit:

$$u \geq 0,$$

$$w \geq 0,$$

$$uw = 0$$

$$\text{on } \Gamma.$$

∂D

Ω

Γ

"Perfectly reflecting or perfectly monitoring"

$$w = 0, \quad u > 0 \quad \text{and} \quad \nabla u \cdot \nu = 0$$

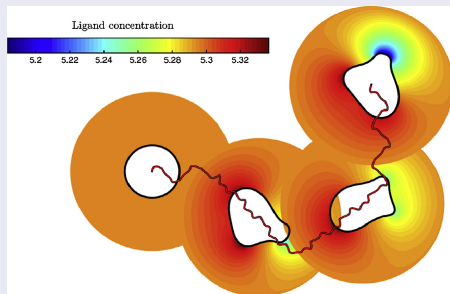
"Perfectly absorbing"

$$u = 0 \quad \text{and} \quad w > 0$$

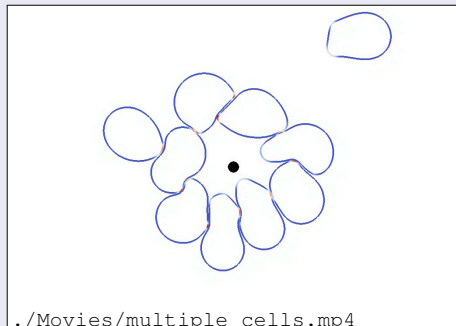
(Endres and Wingreen, 2008)

Systems of coupled bulk-surface PDEs on **evolving domains** arise in a number of models for phenomena in cell biology such as chemotaxis, adhesion, signalling, ...

Chemotaxis

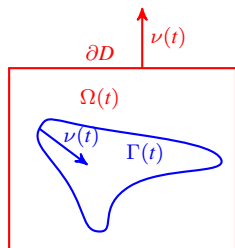


Simulation of single-cell chemotaxis (MacDonald et al., 2016)



Simulation of multi-cell chemotaxis (Elliott, Stinner, and Venkataraman, 2012)

Evolving domain coupled bulk-surface model for receptor-ligand dynamics (Alphonse, Elliott, and Terra, 2018)



- $\mathbf{V}_\Omega$: material velocity of Ω
- $\mathbf{V}_\Gamma$: material velocity of Γ
- $\mathbf{V}_p$: parametrisation velocity field.

Model

$$\mathbf{J}_\Omega := \mathbf{V}_\Omega - \mathbf{V}_p, \quad \mathbf{J}_\Gamma := \mathbf{V}_\Gamma - \mathbf{V}_p \text{ and } j := (\mathbf{V}_\Omega - \mathbf{V}_\Gamma) \cdot \nu.$$

$$\partial^\bullet w := w_t + \nabla w \cdot \mathbf{V}_p$$

$$\delta_\Omega(\partial^\bullet u + u \nabla \cdot \mathbf{V}_p + \nabla \cdot (\mathbf{J}_\Omega u)) - \Delta u = 0 \quad \text{in } \Omega(t)$$

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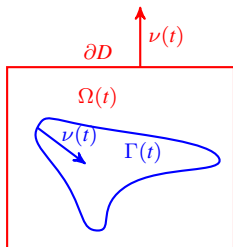
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$$(u(0), w(0), z(0)) = (u_0, w_0, z_0).$$

$\mathbf{V}_p$: not intrinsic to the model but used to define function spaces and relevant to numerics.

$j \neq 0$ corresponds to the so called "windshield effect".

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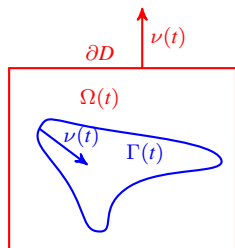
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Theorem (Existence & Uniqueness)

For bounded non-negative data and smooth velocity fields, there exists a unique non-negative weak solution to the evolving domain receptor-ligand system.

- Analysis based on the abstract evolving function space framework of (Alphonse, Elliott, and Stinner, 2015a,b; Vierling, 2014)
- Asymptotic limits and numerics not considered.

Asymptotic limits of an evolving domain coupled bulk-surface model for receptor-ligand dynamics

Model

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$$(u(0), w(0), z(0)) = (u_0, w_0, z_0).$$

$$g(u, w) = uw \quad \text{or} \quad g(u, w) = \frac{u^n w}{1 + u^n} \text{ for } n > 1.$$

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$$\begin{aligned}\delta_{\Omega}(\partial^{\bullet}u + u\nabla \cdot \mathbf{V}_p + \nabla \cdot (\mathbf{J}_{\Omega}u)) - \Delta u &= 0 && \text{in } \Omega(t) \\ \nabla u \cdot \nu - \delta_{\Omega}ju &= \frac{1}{\delta_{k'}}z - \frac{1}{\delta_k}g(u, w) && \text{on } \Gamma(t) \\ u = u_D \text{ or } \nabla u \cdot \nu &= 0 && \text{on } \partial D \\ \partial^{\bullet}w + w\nabla_{\Gamma} \cdot \mathbf{V}_p - \delta_{\Gamma}\Delta_{\Gamma}w + \nabla_{\Gamma} \cdot (\mathbf{J}_{\Gamma}w) &= \frac{1}{\delta_{k'}}z - \frac{1}{\delta_k}g(u, w) && \text{on } \Gamma(t) \\ \partial^{\bullet}z + z\nabla_{\Gamma} \cdot \mathbf{V}_p - \delta_{\Gamma'}\Delta_{\Gamma'}z + \nabla_{\Gamma} \cdot (\mathbf{J}_{\Gamma}z) &= \frac{1}{\delta_k}g(u, w) - \frac{1}{\delta_{k'}}z && \text{on } \Gamma(t) \\ (u(0), w(0), z(0)) &= (u_0, w_0, z_0).\end{aligned}$$

Assumption: Existence & Uniqueness

We take non-negative bounded data and we *assume* the existence of a unique non-negative solution.

(Satisfied in the case $g(u, w) = uw$ from the results of (Alphonse, Elliott, and Terra, 2018))

Fast binding limit: $\delta_k \rightarrow 0$

As $\delta_k \rightarrow 0$, the solution (u_k, w_k, z_k) converges to a weak solution (u, w, z) of the problem

$$\begin{aligned}
 \delta_\Omega (\partial^\bullet u + u \nabla \cdot \mathbf{V}_p + \nabla \cdot (\mathbf{J}_\Omega u)) - \Delta u &= 0 && \text{in } \Omega(t) \\
 \nabla u \cdot \nu &= 0 && \text{on } \partial D \\
 \partial^\bullet w - \delta_\Gamma \Delta_\Gamma w + w \nabla_\Gamma \cdot \mathbf{V}_p + \nabla_\Gamma \cdot (\mathbf{J}_\Gamma w) &= \nabla u \cdot \nu - \delta_\Omega j u && \text{on } \Gamma(t) \\
 \partial^\bullet z - \delta_{\Gamma'} \Delta_{\Gamma'} z + z \nabla_\Gamma \cdot \mathbf{V}_p + \nabla_\Gamma \cdot (\mathbf{J}_\Gamma z) &= -\nabla u \cdot \nu + \delta_\Omega j u && \text{on } \Gamma(t) \\
 g(u, w) &= 0 && \text{on } \Gamma(t) \\
 (u(0), w(0), z(0)) &= (u_0, w_0, z_0).
 \end{aligned}$$

A weak solution is defined to satisfy, for every $\eta \in \mathcal{V}$ with $\eta(T) = 0$,

$$\begin{aligned}
 & - \int_{\Omega_0} u_0 \eta(0) + \frac{1}{\delta_\Omega} \int_{\Gamma_0} w_0 \eta(0) - \int_0^T \int_{\Omega(t)} u \partial^\bullet \eta + \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma} w \partial^\bullet \eta + \frac{1}{\delta_\Omega} \int_0^T \int_{\Omega(t)} \nabla u \cdot \nabla \eta \\
 & - \frac{\delta_\Gamma}{\delta_\Omega} \int_0^T \int_{\Gamma} \nabla_\Gamma w \cdot \nabla_\Gamma \eta + \int_0^T \int_{\Omega(t)} \nabla \cdot (\mathbf{J}_\Omega u) \eta - \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma(t)} \nabla_\Gamma \cdot (\mathbf{J}_\Gamma w) \eta - \int_0^T \int_{\Gamma(t)} j u \eta = 0, \\
 & - \int_{\Omega_0} u_0 \eta(0) - \frac{1}{\delta_\Omega} \int_{\Gamma_0} z_0 \eta(0) - \int_0^T \int_{\Omega(t)} u \partial^\bullet \eta - \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma} z \partial^\bullet \eta + \frac{1}{\delta_\Omega} \int_0^T \int_{\Omega(t)} \nabla u \cdot \nabla \eta \\
 & + \frac{\delta_{\Gamma'}}{\delta_\Omega} \int_0^T \int_{\Gamma} \nabla_\Gamma z \cdot \nabla_\Gamma \eta + \int_0^T \int_{\Omega(t)} \nabla \cdot (\mathbf{J}_\Omega u) \eta + \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma(t)} \nabla_\Gamma \cdot (\mathbf{J}_\Gamma z) \eta - \int_0^T \int_{\Gamma(t)} j u \eta = 0, \\
 & g(u, w) = 0 \text{ on } \Gamma(t).
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 \partial^\bullet w - \delta_\Gamma \Delta_\Gamma w + w \nabla_\Gamma \cdot \mathbf{V}_p + \nabla_\Gamma \cdot (\mathbf{J}_\Gamma w) &= \nabla u \cdot \nu - \delta_\Omega j u && \text{on } \Gamma(t) \\
 \partial^\bullet z - \delta_{\Gamma'} \Delta_{\Gamma'} z + z \nabla_\Gamma \cdot \mathbf{V}_p + \nabla_\Gamma \cdot (\mathbf{J}_\Gamma z) &= -\nabla u \cdot \nu + \delta_\Omega j u && \text{on } \Gamma(t) \\
 g(u, w) &= 0 && \text{on } \Gamma(t) \\
 (u(0), w(0), z(0)) &= (u_0, w_0, z_0).
 \end{aligned}$$

A weak solution is defined to satisfy, for every $\eta \in \mathcal{V}$ with $\eta(T) = 0$,

$$\begin{aligned}
 & - \int_{\Omega_0} u_0 \eta(0) + \frac{1}{\delta_\Omega} \int_{\Gamma_0} w_0 \eta(0) - \int_0^T \int_{\Omega(t)} u \partial^\bullet \eta + \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma} w \partial^\bullet \eta + \frac{1}{\delta_\Omega} \int_0^T \int_{\Omega(t)} \nabla u \cdot \nabla \eta \\
 & - \frac{\delta_\Gamma}{\delta_\Omega} \int_0^T \int_{\Gamma} \nabla_\Gamma w \cdot \nabla_\Gamma \eta + \int_0^T \int_{\Omega(t)} \nabla \cdot (\mathbf{J}_\Omega u) \eta - \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma(t)} \nabla_\Gamma \cdot (\mathbf{J}_\Gamma w) \eta - \int_0^T \int_{\Gamma(t)} j u \eta = 0, \\
 & - \int_{\Omega_0} u_0 \eta(0) - \frac{1}{\delta_\Omega} \int_{\Gamma_0} z_0 \eta(0) - \int_0^T \int_{\Omega(t)} u \partial^\bullet \eta - \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma} z \partial^\bullet \eta + \frac{1}{\delta_\Omega} \int_0^T \int_{\Omega(t)} \nabla u \cdot \nabla \eta \\
 & + \frac{\delta_{\Gamma'}}{\delta_\Omega} \int_0^T \int_{\Gamma} \nabla_{\Gamma'} z \cdot \nabla_{\Gamma'} \eta + \int_0^T \int_{\Omega(t)} \nabla \cdot (\mathbf{J}_\Omega u) \eta + \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma(t)} \nabla_\Gamma \cdot (\mathbf{J}_\Gamma z) \eta - \int_0^T \int_{\Gamma(t)} j u \eta = 0, \\
 & g(u, w) = 0 \text{ on } \Gamma(t).
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Fast binding, slow surface diffusion limit: $\delta_k = \delta_\Gamma = \delta_{\Gamma'} \rightarrow 0$

As $\delta_k = \delta_\Gamma = \delta_{\Gamma'} \rightarrow 0$, the solution (u_k, w_k, z_k) converges to a weak solution (u, w, z) of the problem

$$\begin{aligned}
 \delta_\Omega(\partial^\bullet u + u \nabla_\Gamma \cdot \mathbf{V}_p + \nabla \cdot (\mathbf{J}_\Omega u)) - \Delta u &= 0 && \text{in } \Omega(t) \\
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 \partial^\bullet w + w \nabla_\Gamma \cdot \mathbf{V}_p + \nabla_\Gamma \cdot (\mathbf{J}_\Gamma w) &= \nabla u \cdot \nu - \delta_\Omega j u && \text{on } \Gamma(t) \\
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 & + \int_0^T \int_{\Omega(t)} \nabla \cdot (\mathbf{J}_\Omega u) \eta + \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma(t)} w \mathbf{J}_\Gamma \cdot \nabla_\Gamma \eta - \int_0^T \int_{\Gamma(t)} j u \eta = 0, \\
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 & + \int_0^T \int_{\Omega(t)} \nabla \cdot (\mathbf{J}_\Omega u) \eta - \frac{1}{\delta_\Omega} \int_0^T \int_{\Gamma(t)} z \mathbf{J}_\Gamma \cdot \nabla_\Gamma \eta - \int_0^T \int_{\Gamma(t)} j u \eta = 0, \\
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Fast binding, slow surface diffusion limit: $\delta_k = \delta_\Gamma = \delta_{\Gamma'} \rightarrow 0$

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$$\delta_k = \delta_\Gamma = \delta_{\Gamma'} = \delta_\Omega = \delta_k^{-1} \rightarrow 0 \text{ limit}$$

Assume that $\mathbf{J}_\Gamma \equiv 0$. As $\delta_\Omega = \delta_k = \frac{1}{\delta_k'} = \delta_\Gamma = \delta_{\Gamma'} \rightarrow 0$, the solution (u_k, w_k, z_k) converges to a weak solution (u, w, z) of the problem

$$\begin{aligned} \Delta u &= 0 && \text{in } \Omega(t) \\ u &= u_D && \text{on } \partial D \\ \partial^\bullet w + w \nabla_\Gamma \cdot \mathbf{V}_\Gamma &= \nabla u \cdot \nu && \text{on } \Gamma(t) \\ \partial^\bullet z + z \nabla_\Gamma \cdot \mathbf{V}_\Gamma &= -\nabla u \cdot \nu && \text{on } \Gamma(t) \\ g(u, w) &= 0 && \text{on } \Gamma(t) \\ (w(0), z(0)) &= (w_0, z_0). \end{aligned}$$

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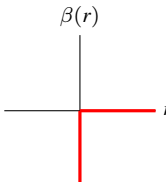
$$\begin{aligned} \Delta u &= 0 && \text{in } \Omega(t) \\ u &= u_D && \text{on } \partial D \\ \partial^\bullet w + w \nabla_\Gamma \cdot \mathbf{V}_\Gamma &= \nabla u \cdot \nu && \text{on } \Gamma(t) \\ \partial^\bullet z + z \nabla_\Gamma \cdot \mathbf{V}_\Gamma &= -\nabla u \cdot \nu && \text{on } \Gamma(t) \\ g(u, w) &= 0 && \text{on } \Gamma(t) \\ (w(0), z(0)) &= (w_0, z_0). \end{aligned}$$

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Formulation as Stefan-type free boundary problems on evolving surfaces

If we define $v := -w$ and define the maximal monotone graph β by

$$\beta(r) := \begin{cases} \emptyset & : r < 0 \\ (-\infty, 0] & : r = 0 \\ 0 & : r > 0 \end{cases}$$


we can recast the condition $u, w \geq 0, g(u, w) = 0$ on $\Gamma(t)$ as $v \in \beta(u)$ on $\Gamma(t)$.

Defining $P: L^2_{H^{1/2}(\Gamma)} \rightarrow L^2_{H^1(\Omega)}$ the solution map $u \mapsto U$ of

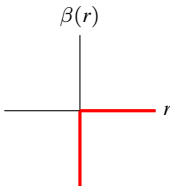
$$\begin{aligned} \delta_\Omega(\partial^\bullet U + U \nabla \cdot \mathbf{V}_p + \nabla \cdot (\mathbf{J}_\Omega U)) - \Delta U &= 0 && \text{in } \Omega(t) \\ \nabla U \cdot \nu &= 0 && \text{on } \partial D \\ U &= u && \text{on } \Gamma(t) \\ U(0) &= u_0 && \text{on } \Omega_0 \end{aligned}$$

and define the associated Dirichlet-to-Neumann map $A: L^2_{H^{1/2}(\Gamma)} \rightarrow L^2_{H^{-1/2}(\Gamma)}$ by

$$A(u) := \nabla P(u) \cdot \nu.$$

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Formulation as Stefan-type free boundary problems on evolving surfaces

$\delta_k \rightarrow 0$ limit. We can rewrite the problem as: find (u, v) with $u \geq 0, v \leq 0$, such that

$$\begin{aligned}\partial^\bullet v - \delta_\Gamma \Delta_\Gamma v + v \nabla_\Gamma \cdot \mathbf{V}_p + \nabla_\Gamma \cdot (\mathbf{J}_\Gamma v) + A(u) &= \delta_\Omega j u && \text{on } \Gamma(t) \\ v &\in \beta(u) \\ v(0) &= v_0\end{aligned}$$

$\delta_k = \delta_\Gamma = \delta_{\Gamma'} \rightarrow 0$ limit. We can rewrite the problem as: find (u, v) with $u \geq 0, v \leq 0$, such that

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$\delta_\Omega = \delta_k = \delta_{k'}^{-1} = \delta_\Gamma = \delta_{\Gamma'} \rightarrow 0$ limit. We can rewrite the problem as: find (u, v) with $u \geq 0, v \leq 0$ such that

$$\begin{aligned}\partial^\bullet v + v \nabla_\Gamma \cdot \mathbf{V}_\Gamma + A_D(u) + \nabla h \cdot \nu &= 0 && \text{on } \Gamma(t) \\ v &\in \beta(u) \\ v(0) &= v_0\end{aligned}$$

Approach for uniqueness used in fixed domain setting (Elliott, Ranner, and Venkataraman, 2017) *not* directly applicable.

Formulation as Stefan-type free boundary problems on evolving surfaces

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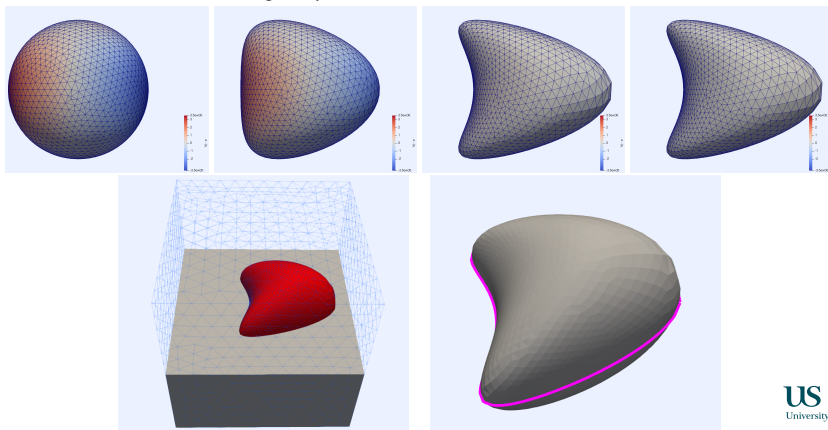
$$\begin{aligned}\partial^\bullet v + v \nabla_\Gamma \cdot \mathbf{V}_p + \nabla_\Gamma \cdot (\mathbf{J}_\Gamma v) + A(u) &= \delta_\Omega j u && \text{on } \Gamma(t) \\ v &\in \beta(u) \\ v(0) &= v_0\end{aligned}$$

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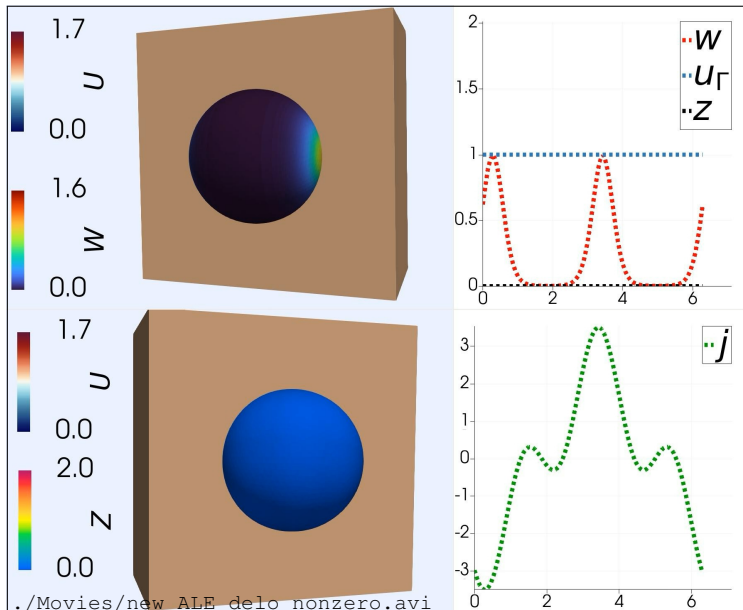
$$\begin{aligned}\partial^\bullet v + v \nabla_\Gamma \cdot \mathbf{V}_\Gamma + A_D(u) + \nabla h \cdot \nu &= 0 && \text{on } \Gamma(t) \\ v &\in \beta(u) \\ v(0) &= v_0\end{aligned}$$

Approach for uniqueness used in fixed domain setting (Elliott, Ranner, and Venkataraman, 2017) *not* directly applicable.

- $D = [-2, 2]^3$
- $\Gamma(t)$ defined as the zero level set of $\phi(\mathbf{x}, t) = \left(x_1 + \tanh(5t) (0.7 - x_2^2) \right)^2 + x_2^2 + x_3^2 - 1$.
- We set $\mathbf{V}_\Gamma = V\boldsymbol{\nu}$.
- We take $\mathbf{V}_\Omega = \mathbf{0}$ (windshield effect) or $\mathbf{V}_\Omega = E(\mathbf{V}_\Gamma)$ (no windshield effect)
- We set $u_0 = u_D = 1, z_0 = 0$
- Numerics based on an evolving coupled bulk-surface FEM.



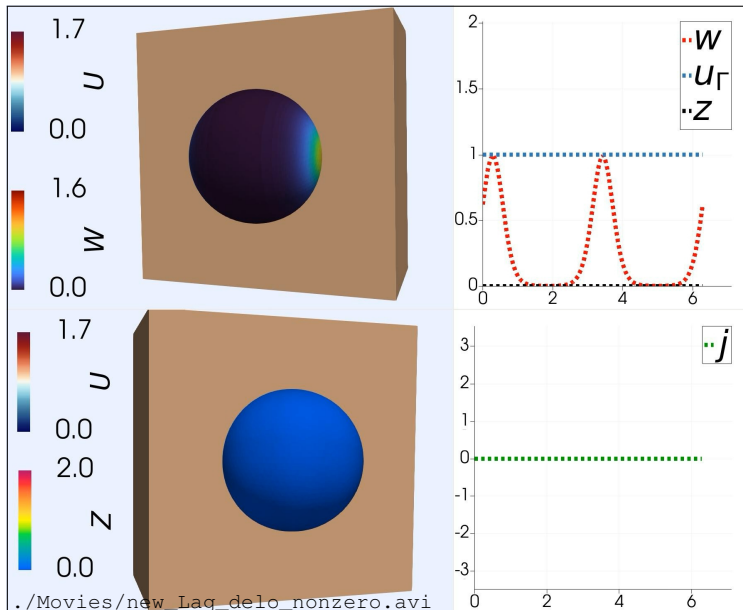
$$\delta_k = \delta_\Gamma = \delta_{\Gamma'} = 0.001, \quad \mathbf{V}_\Omega = 0, \quad g(u, w) = \frac{u^2}{1+u^2} w$$



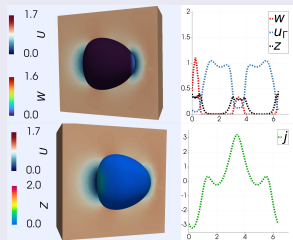
$$\delta_k = \delta_\Gamma = \delta_{\Gamma'} = 0.001,$$

$$\mathbf{V}_\Omega = E(\mathbf{V}_\Gamma),$$

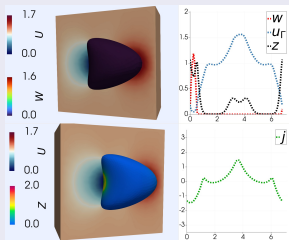
$$g(u, w) = \frac{u^2}{1+u^2} w$$



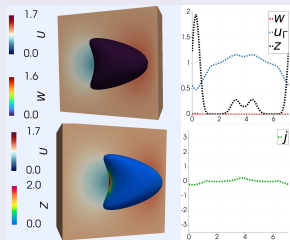
$$V_{\Omega} = 0$$



(a) $t = 0.06$

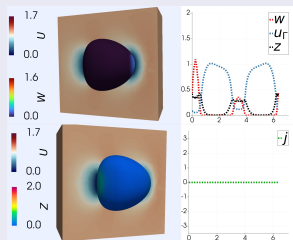


(b) $t = 0.2$

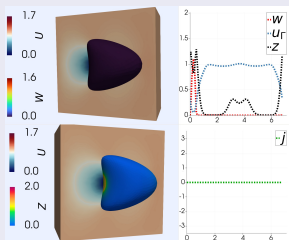


(c) $t = 0.4$

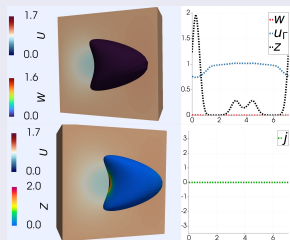
$$V_{\Omega} = E(V_{\Gamma})$$



(d) $t = 0.06$



(e) $t = 0.2$

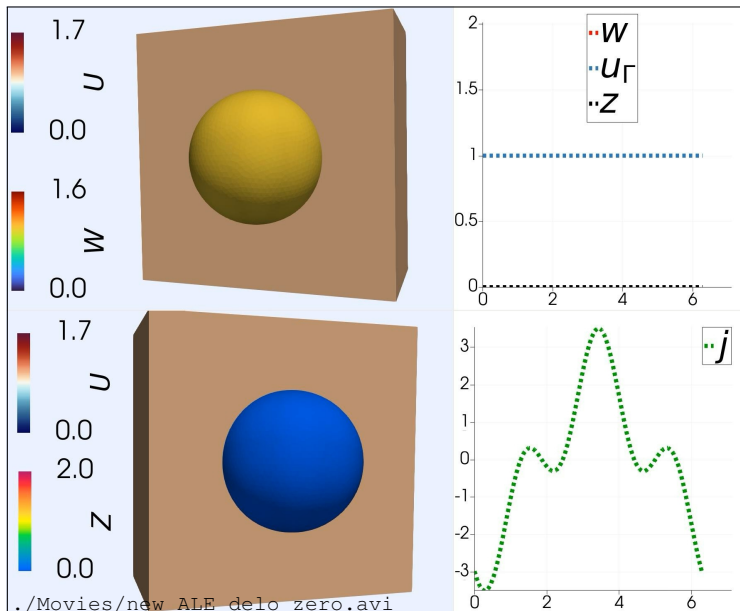


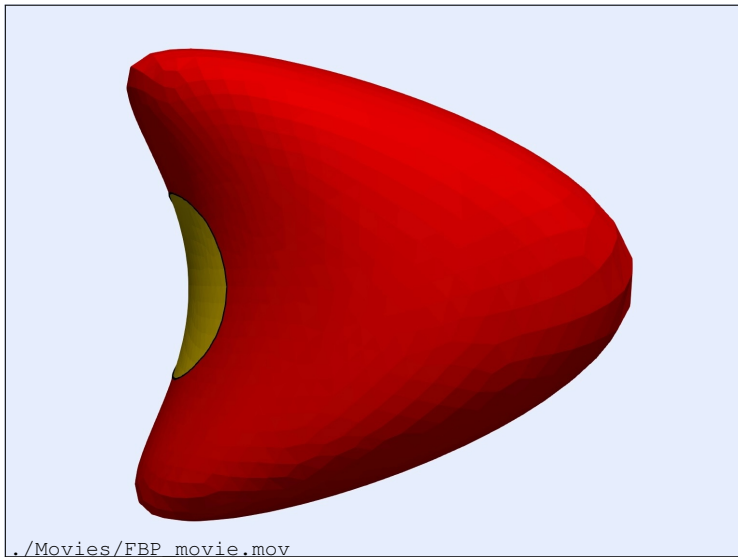
(f) $t = 0.4$

$$\delta_k = \delta_\Gamma = \delta_{\Gamma'} = \delta_\Omega = \delta_{k'}^{-1} = 0.01,$$

$$\mathbf{V}_\Omega = 0,$$

$$g(u, w) = uw$$





Summary

- Asymptotic limits of models for receptor-ligand interactions on *evolving domains*.
- Limiting problems correspond to Stefan-type free boundary problems on an evolving surface.
- Numerics illustrating the free boundary and effects due to domain evolution.

Outlook

- Uniqueness for the limiting problems (vanishing surface diffusion cases).
- Numerics for the limiting problems (vanishing surface diffusion cases).
- Coupling to biochemistry in cell bulk.
- Coupling to (unknown) surface evolution.

References:

CM Elliott, T Ranner and C Venkataraman. "Coupled bulk-surface free boundary problems arising from a mathematical model of receptor-ligand dynamics". *SIAM J. Math. Anal.* 2017

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A Alphonse, D Caetano, CM Elliott, and C Venkataraman. "Free boundary limits of coupled bulk surface models for receptor-ligand interactions on evolving domains". *in prep*

Thank You

