Finite Volume Methods for Advection Diffusion on Moving Interfaces and Application on Surfactant Driven Thin Film Flow

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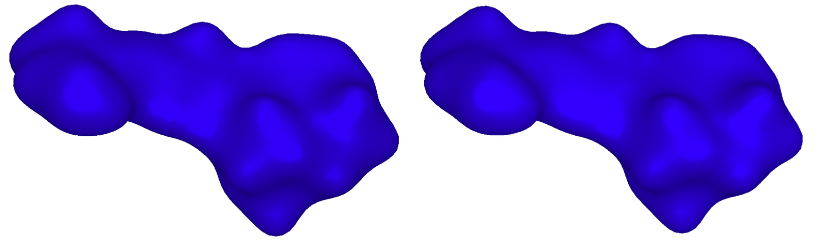
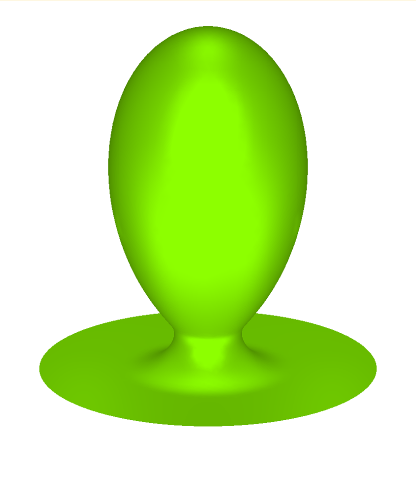
Outline

- Advection-Diffusion-Reaction on surfaces



- Thin-film flow in a lung alveolus

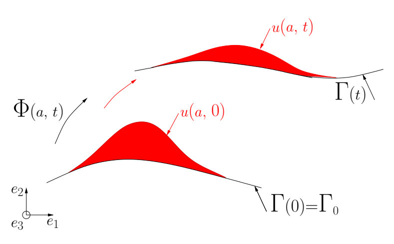


Problem Formulation

$\Gamma(t)$: Family of 2-d smooth surfaces

$\Phi(\cdot, t)$: Sufficiently smooth map, $\Phi(\Gamma(0), t) = \Gamma(t)$

$u(a, t)$: density of a scalar quantity on $\Gamma(t)$



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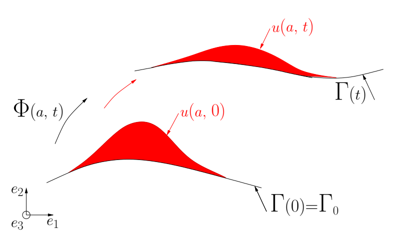

Find $u(\cdot,\, t)$ such that

$$\dot{u} + u\nabla_{\Gamma(t)} \cdot v_\Gamma - \nabla_{\Gamma(t)} \cdot \left(\mathcal{D}_0 \nabla_{\Gamma(t)} u\right) = g \quad \text{on } \Gamma(t)$$

$$u(\cdot,\, 0) = u_0(\cdot) \quad \text{on } \Gamma_0$$

$+$BC

$v_\Gamma(\cdot,\, t)$: Velocity field on $\Gamma(t)$, $\quad g$: source term

$\mathcal{D}_0$: Symmetric elliptic diffusion tensor on the tangent plane

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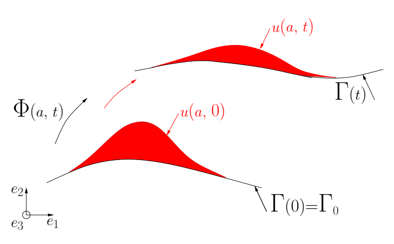

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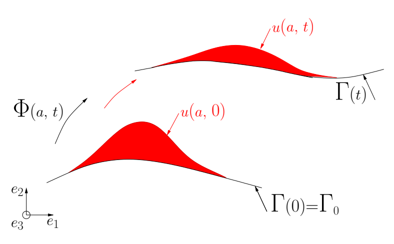

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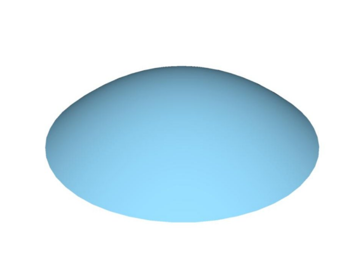
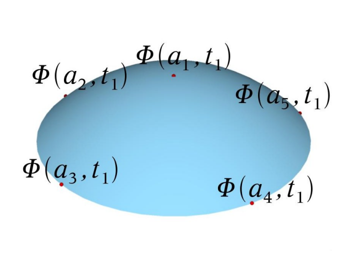
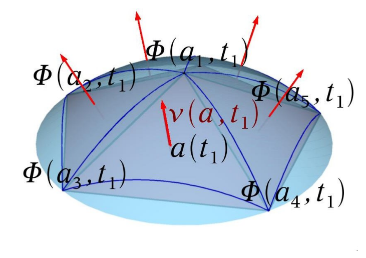
Two points flux approximation Finite Volumes (Discretization)

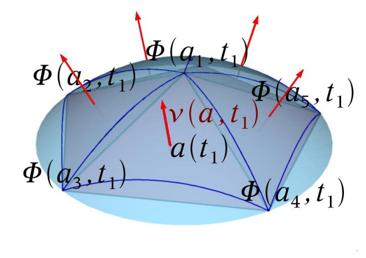


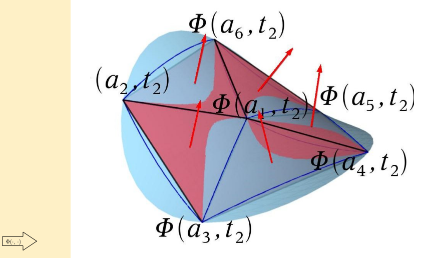


$\Phi(a_1, t_1)$
$\Phi(a_2, t_1)$
$\Phi(a_5, t_1)$
$\Phi(a_3, t_1)$
$\Phi(a_4, t_1)$



$$x(t) = a(t) - d(a(t))\nu(a(t))$$





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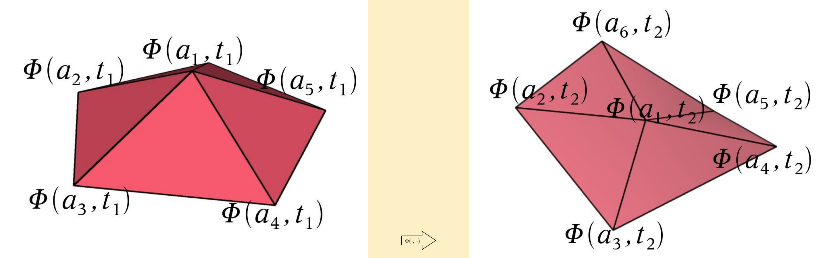

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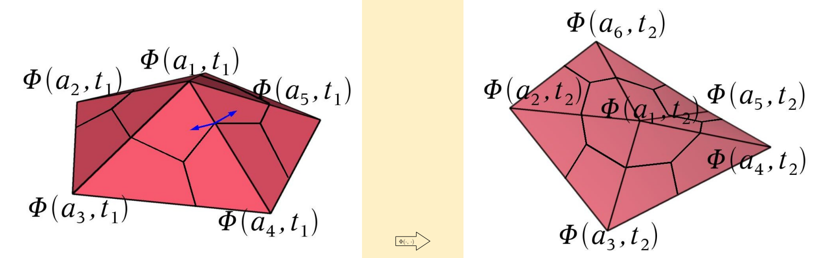
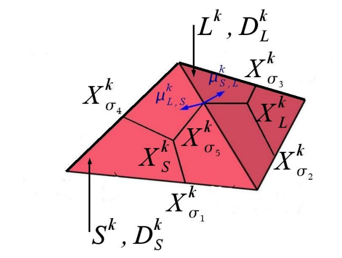
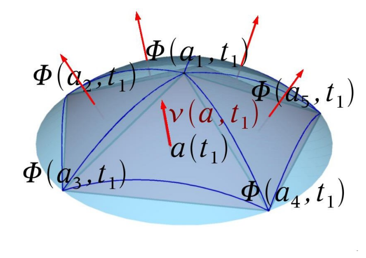
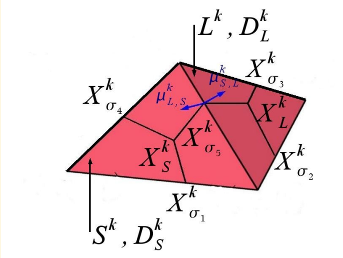


$Zoom$ of two cells at t_k



For the simplicity, we assume $\mathcal{D} = \mathcal{I}_d$





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$$\int_{t_k}^{t_{k+1}} \int_{S^l(t)} \left(\dot{u} + u \nabla_{\Gamma(t)} \cdot v_\Gamma \right) - \int_{t_k}^{t_{k+1}} \int_{S^l(t)} \nabla \cdot (\mathcal{D}_0 \nabla u)$$

$$= \int_{t_k}^{t_{k+1}} \int_{S^l(t)} g$$

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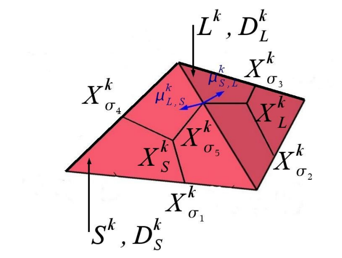

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$$\int_{t_k}^{t_{k+1}} \int_{S^l(t)} \left(\dot{u} + u \nabla_{\Gamma(t)} \cdot v_\Gamma \right) = \int_{t_k}^{t_{k+1}} \frac{d}{dt} \int_{S^l(t)} u$$

$$\approx m(S(t_{k+1}))\, u_S^{k+1} - m(S(t_k))\, u_S^k$$

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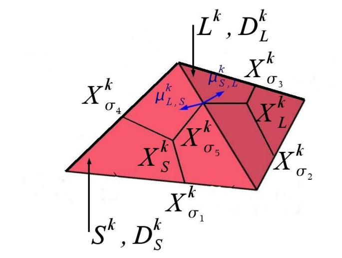

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$$\underbrace{-\int_{t_k}^{t_{k+1}} \int_{S^l(t)} \nabla \cdot (\mathcal{D}_0 \nabla u)}_{\approx}$$

$$\tau \sum_{\sigma_i \subset \partial S(t_{k+1})} m(\sigma_i) \frac{u_{\sigma_i}^{k+1} - u_S^{k+1}}{\| \overrightarrow{X_S^{k+1} X_{\sigma_i}^{k+1}} \|}$$

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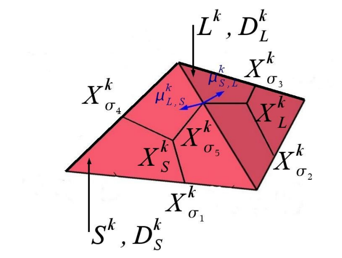
$Zoom$ of two cells at t_k



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$\Longrightarrow$ Using flux balance at interfaces

$$\tau \sum_{\sigma_i \subset \partial S} m(\sigma_i) \frac{1}{\| \overrightarrow{X_S^{k+1} X_{\sigma_i}^{k+1}} \| + \| \overrightarrow{X_{L_i}^{k+1} X_{\sigma_i}^{k+1}} \|} \cdot (u_{L_i}^{k+1} - u_S^{k+1})$$

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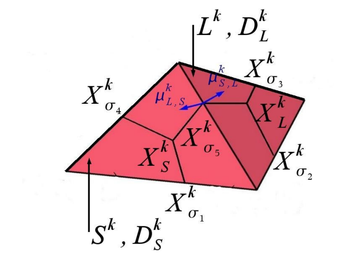

$$\int_{t_k}^{t_{k+1}} \int_{S^l(t)} g \quad \approx \quad \tau m(S(t_{k+1})) g_S^{k+1}$$

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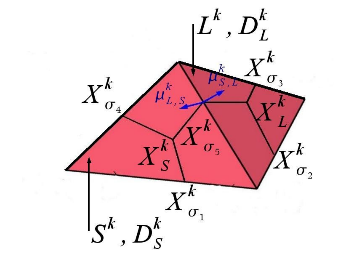

Find $\left\{ u_S^{k+1} \right\}_{S,\,k}$ **such that:**

$$m(S(t_{k+1}))\, u_S^{k+1} - m(S(t_k))\, u_S^k$$

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Interpretation:

$$u^k = \left\{ u_S^k \right\} \equiv \sum_S u_S^k \chi_S$$

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Discrete H_0^1 **semi-norm:** $\displaystyle\sum_{\sigma_i = S(t_k)|L(t_k)} m(\sigma_i) \frac{1}{\| \overrightarrow{X_S^k\, X_{\sigma_i}^k} \| + \| \overrightarrow{X_L^k\, X_{\sigma_i}^k} \|} \cdot \left(u_L^k - u_S^k\right)^2$

Discrete $\mathbb{L}^2$ **norm:** $\|U^k\|^2_{\mathbb{L}^2(\Gamma_h^k)} := \sum_S m(S(t_k)) \left(U_S^k\right)^2$

Theorem: The above system has a unique solution

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Proposition 1: Stability, $\mathbb{L}^\infty(\mathbb{L}^2)$ and $\mathbb{L}^2(\mathbb{H}_0^1)$

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Proposition 2: Stability, $\mathbb{L}^2(\mathbb{L}^2)$ for $\partial_\tau U = \frac{U^{k+1}-U^k}{\tau}$, $\mathbb{L}^\infty(\mathbb{H}_0^1)$ for U

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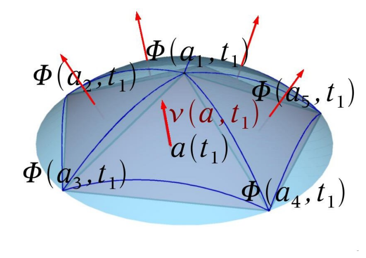
Theorem:

u: Real solution on $\Gamma(t)$,

u^k: Discrete solution on $\Gamma_h(t_k)$

$$E^k = \sum_S \left(u^{-l}\left(X_S^k, t_k\right) - u_S^k\right)\chi_S$$

$$\| E^k \|_{\mathbb{L}^2(\Gamma_h(t_k))} \leq C\,(h + \tau)$$



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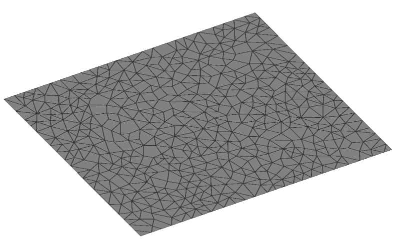
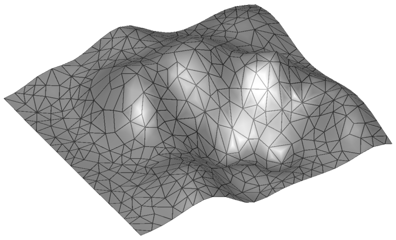
O-Method Finite

polygonal surface

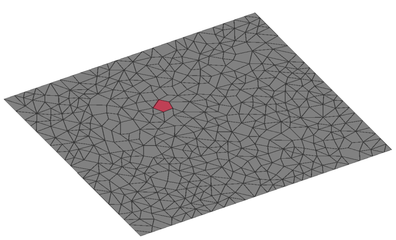


Initial surface (plane)



Evolved surface

polygonal surface



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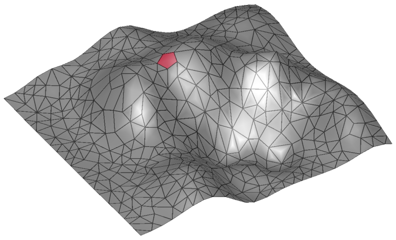

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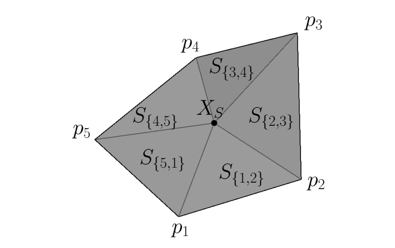
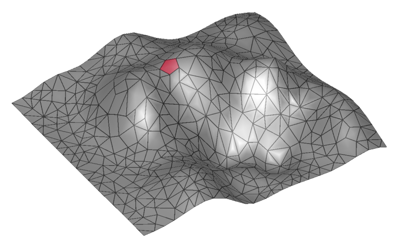


Cell



Evolved surface

Definition (Cell):

Given vertices p_i $(i = 1, \cdots, n_S)$ and a center point X_S, the cell S is the closed fan of triangles $S_{\{i,i+1\}} = [X_S, p_i, p_{i+1}]$ $(i + 1 \equiv (i \bmod n_S) + 1)$.

Problem setup

Unknown function:

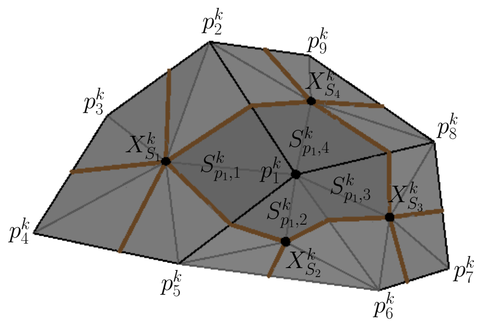
$u(\cdot, t_k)$ sufficiently smooth on $\Gamma^k = \Gamma(t_k)$, extended in $\mathcal{N}_{\delta,k} = \Phi(\mathcal{N}_{\delta,0}, t_k)$ such that $\nabla u(\cdot, t_k) \cdot \nabla d(\cdot, \Gamma^k) \equiv 0$.

Known:

U_S, values of u at cell center X_S, $+$ BC.

Approximate function:

Affine on subcells S_{p_i}; thus constant gradient on subcells S_{p_i}.



Subdivision of cells and renumbering around the vertex p_1^k

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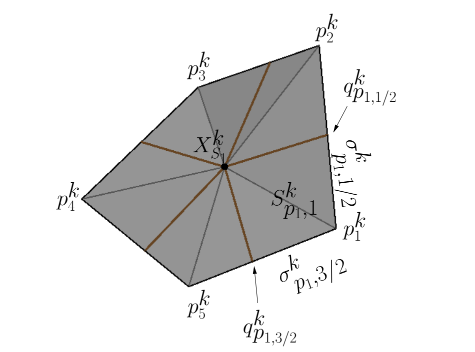


Zoom into a single cell

Geometric setup

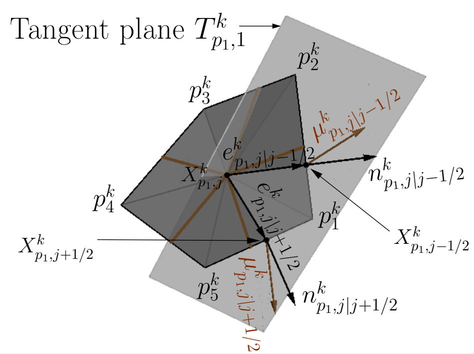
Local covariant basis:

$(e^k_{p_1,j|j+1/2}, e^k_{p_1,j|j-1/2})$

Local contravariant (dual) basis:

$(\mu^k_{p_1,j|j+1/2}, \mu^k_{p_1,j|j-1/2})$

$\mu^k_{p_1,j|j+l/2} \cdot e^k_{p_1,j|j+k/2} = \delta^l_k$, $l \in \{-1,1\}$.



Geometric setup on subcells

Unit outward conormals: $n^k_{p_1,j|j+1/2}$, and $n^k_{p_1,j|j-1/2} \in T^k_{p_1,j}$

$$n^k_{p_1,j|j+1/2} \cdot \overrightarrow{p^k_1 p^k_5} = 0, \quad n^k_{p_1,j|j-1/2} \cdot \overrightarrow{p^k_1 p^k_2} = 0$$

Projection onto the tangent plane $T^k_{p_1,j}$: $\mathcal{P}^k_{p_1,j}$

Approximation on subcells

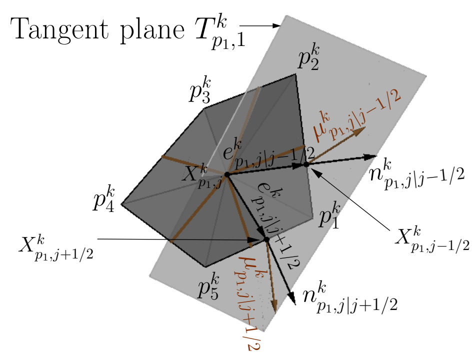
Diffusion tensor:

$$\mathcal{D} \approx \mathcal{D}^k_{p_1,j} := \mathcal{P}^k_{p_1,j}\mathcal{D}\mathcal{P}^k_{p_1,j}$$

Gradient:

$$\nabla_\Gamma u \approx \nabla^k_{p_1,j} u$$
$$:= (U^k_{p_1,j+1/2} - U^k_{p_1,j})\mu^k_{p_1,j|j+1/2}$$
$$+ (U^k_{p_1,j-1/2} - U^k_{p_1,j})\mu^k_{p_1,j|j-1/2}$$

$$\mathcal{D}\nabla_\Gamma u \approx \mathcal{D}^k_{p_1,j}\nabla^k_{p_1,j} u$$



Geometric setup on subcells

$$\Longrightarrow \quad m^k_{p_1,j-1/2}\left(\mathcal{D}^k_{p_1,j-1}\nabla^k_{p_1,j-1}u\right)\cdot n^k_{p_1,j-1|j-1/2} = -m^k_{p_1,j-1/2}\left(\mathcal{D}^k_{p_1,j}\nabla^k_{p_1,j}u\right)\cdot n^k_{p_1,j|j-1/2}, \quad + BC \text{ if necessary}$$

$$m^k_{p_1,j-1/2} = \|\overrightarrow{q^k_{p_1,j-1/2}p^k_i}\|$$

Gradient reconstruction

$$\Longrightarrow \begin{array}{l} m^k_{p_1,j-1/2}\left(\mathcal{D}^k_{p_1,j-1}\nabla^k_{p_1,j-1}u\right)\cdot n^k_{p_1,j-1|j-1/2} \\ = -m^k_{p_1,j-1/2}\left(\mathcal{D}^k_{p_1,j}\nabla^k_{p_1,j}u\right)\cdot n^k_{p_1,j|j-1/2}, \end{array} \qquad + BC \text{ if necessary}$$

$$\Longrightarrow M^k_{p_1}\widetilde{U}^k_{p_1,\sigma} = N^k_{p_1}\widetilde{U}^k_{p_1}$$

$\widetilde{U}^k_{p_1,\sigma} := (U^k_{p_1,1/2}, U^k_{p_1,3/2}, \cdots)^\top$, $\widetilde{U}^k_{p_1} := (U^k_{p_1,1}, U^k_{p_1,2}, \cdots)^\top$

Stabilization of the gradient:

$$\begin{cases} \text{Find } \widetilde{U}^k_{p_1,\sigma} \text{ in } \mathcal{B}^k_{p_1} := \{\widetilde{V}^k_{p_1,\sigma} := (V^k_{p_1,1/2}, V^k_{p_1,3/2}, \cdots)^\top \mid M^k_{p_1}\widetilde{V}^k_{p_1,\sigma} = N^k_{p_1}\widetilde{U}^k_{p_1}\} \text{ such that} \\ \widetilde{U}^k_{p_1,\sigma} = \underset{\widetilde{V}^k_{p_1,\sigma}\in\mathcal{B}^k_{p_1}}{\operatorname{argmin}} \sum_j m^k_{p_1,j} \left\| \left[V^k_{p_1,j-1/2} - U^k_{p_1,j}\right]\mu^k_{p_1,j|j-1/2} + \left[V^k_{p_1,j+1/2} - U^k_{p_1,j}\right]\mu^k_{p_1,j|j+1/2} \right\|^2, \end{cases}$$

where $m^k_{p_1,j} := m(S^k_{p_1,j})$ approximates $m(S^{l,k}_{p_1,j})$.

Gradient reconstruction

$$\Longrightarrow \quad \begin{aligned} & m^k_{p_1,j-1/2}\left(\mathcal{D}^k_{p_1,j-1}\nabla^k_{p_1,j-1}u\right)\cdot n^k_{p_1,j-1|j-1/2} \\ &= -m^k_{p_1,j-1/2}\left(\mathcal{D}^k_{p_1,j}\nabla^k_{p_1,j}u\right)\cdot n^k_{p_1,j|j-1/2}, \qquad + BC \text{ if necessary} \end{aligned}$$

$$\Longrightarrow M^k_{p_1}\widetilde{U}^k_{p_1,\sigma} = N^k_{p_1}\widetilde{U}^k_{p_1}$$

$\widetilde{U}^k_{p_1,\sigma} := (U^k_{p_1,1/2}, U^k_{p_1,3/2}, \cdots)^\top, \quad \widetilde{U}^k_{p_1} := (U^k_{p_1,1}, U^k_{p_1,2}, \cdots)^\top$

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$$\Longrightarrow \widetilde{U}^k_{p_1,\sigma} \;=\; \mathbf{Coef}^k_{p_1}\widetilde{U}^k_{p_1}$$

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where $m^k_{p_1,j} := m(S^k_{p_1,j})$ approximates $m(S^{l,k}_{p_1,j})$.

$$\Longrightarrow \widetilde{U}^k_{p_1,\sigma} = \mathbf{Coef}^k_{p_1}\widetilde{U}^k_{p_1}$$

$M^k_{p_1}$ invertible $\Longrightarrow \mathbf{Coef}^k_{p_1} = \left(M^k_{p_1}\right)^{-1} N^k_{p_1}$

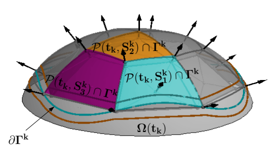
O-Method Finite Volumes (Discretization)

Find $u(\cdot, t)$ such that

$$\dot{u} + u\nabla_{\Gamma(t)} \cdot v - \nabla_{\Gamma(t)} \cdot \left(\mathcal{D}_0 \nabla_{\Gamma(t)} u\right) = g \quad \text{on } \Gamma(t)$$

$$u(\cdot, 0) = u_0(\cdot) \quad \text{on } \Gamma_0$$

+BC



Representation of $\mathcal{P}(S_j^k, t_k) \cap \Gamma^k$ $(j = 1, 2, 3)$

$$\int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} \left(\dot{u} + u\,\nabla_{\Gamma(t)} \cdot v_\Gamma\right) - \int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} \nabla \cdot (\mathcal{D}_0 \nabla u)$$

$$= \int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} g$$

$$S^{l,k}(t) := \Phi(\Phi^{-1}(S^{l,k}, t_k), t), \qquad S^{l,k} := \mathcal{P}(S^k, t_k)$$

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$$\dot{u} + u\nabla_{\Gamma(t)} \cdot v_\Gamma - \nabla_{\Gamma(t)} \cdot \left(\mathcal{D}_0 \nabla_{\Gamma(t)} u\right) = g \quad \text{on } \Gamma(t)$$

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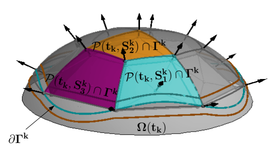

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$$= \int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} g$$

$$S^{l,k}(t) := \Phi(\Phi^{-1}(S^{l,k}, t_k), t), \qquad S^{l,k} := \mathcal{P}(S^k, t_k)$$

$$\int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} g \quad \approx \quad \tau\, m_S^{k+1} G_S^{k+1} \quad ,$$

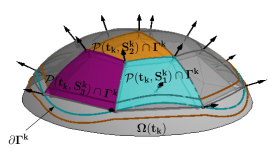
$$G_S^{k+1} := g\left(t, \mathcal{P}^{k+1} X_S^{k+1}\right).$$

Find $u(\cdot, t)$ such that

$\dot{u} + u\nabla_{\Gamma(t)} \cdot v_\Gamma - \nabla_{\Gamma(t)} \cdot \left(\mathcal{D}_0 \nabla_{\Gamma(t)} u\right) = g$ on $\Gamma(t)$

$u(\cdot, 0) = u_0(\cdot)$ on Γ_0

+BC



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$$\int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} \left(\dot{u} + u\,\nabla_{\Gamma(t)} \cdot v_\Gamma\right) - \int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} \nabla \cdot (\mathcal{D}_0 \nabla u)$$

$$= \int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} g$$

$$\int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} (\dot{u} + u\nabla_\Gamma v_\Gamma)$$

$$= \int_{S^{l,k}(t_{k+1})\cap\Gamma(t_{k+1})} u - \int_{S^{l,k}(t_k)\cap\Gamma(t_k)} u \quad \approx \quad m_S^{k+1} U_S^{k+1} - m_S^k U_S^k.$$

Find $u(\cdot, t)$ such that

$$\dot{u} + u\nabla_{\Gamma(t)} \cdot v_\Gamma - \nabla_{\Gamma(t)} \cdot \left(\mathcal{D}_0 \nabla_{\Gamma(t)} u\right) = g \quad \text{on } \Gamma(t)$$

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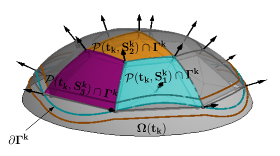

Representation of $\mathcal{P}(S_j^k, t_k) \cap \Gamma^k$ $(j = 1, 2, 3)$

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$$= \int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} g$$

$$\int_{t_k}^{t_{k+1}} \int_{S^{l,k}(t)\cap\Gamma(t)} \nabla_\Gamma \cdot (\mathcal{D}\nabla_\Gamma u) = \int_{t_k}^{t_{k+1}} \int_{\partial(S^{l,k}(t)\cap\Gamma(t))} (\mathcal{D}\nabla_\Gamma u) \cdot \mu_{\partial S^{l,k}(t)}$$

$$\approx \tau \sum_{p_i \in \partial S^k} \Big(m^{k+1}_{p_i,\mathcal{J}(p_i,S^k)-1/2} \mathcal{D}^k_{p_i,\mathcal{J}(p_i,S^k)} \nabla^{k+1}_{p_i,\mathcal{J}(p_i,S^k)} u \cdot n^{k+1}_{p_i,\mathcal{J}(p_i,S^k)|\mathcal{J}(p_i,S^k)-1/2}$$

$$+ \; m^{k+1}_{p_i,\mathcal{J}(p_i,S^k)+1/2} \mathcal{D}^k_{p_i,\mathcal{J}(p_i,S^k)} \nabla^{k+1}_{p_i,\mathcal{J}(p_i,S^k)} u \cdot n^{k+1}_{p_i,\mathcal{J}(p_i,S^k)|\mathcal{J}(p_i,S^k)+1/2} \Big).$$

$\mathcal{J}(p_i, S^k)$: local index number of the cell S^k around p_i^k.

Discrete problem:

Find $\left\{U_S^k\right\}_{S,k}$ such that:

$$
\begin{aligned}
& m_S^{k+1}U_S^{k+1} - m_S^k U_S^k - \tau \sum_{p_i \in \partial S^k} \\
& \Big(m^{k+1}_{p_i,\mathcal{J}(p_i,S^k)-1/2} \mathcal{D}^k_{p_i,\mathcal{J}(p_i,S^k)} \nabla^{k+1}_{p_i,\mathcal{J}(p_i,S^k)} u \cdot n^{k+1}_{p_i,\mathcal{J}(p_i,S^k)|\mathcal{J}(p_i,S^k)-1/2} \\
+ \quad & m^{k+1}_{p_i,\mathcal{J}(p_i,S^k)+1/2} \mathcal{D}^k_{p_i,\mathcal{J}(p_i,S^k)} \nabla^{k+1}_{p_i,\mathcal{J}(p_i,S^k)} u \cdot n^{k+1}_{p_i,\mathcal{J}(p_i,S^k)|\mathcal{J}(p_i,S^k)+1/2} \Big) \\
= \quad & \tau\, m_S^{k+1} G_S^{k+1},
\end{aligned}
$$

$$
U_S^0 := u(t_0, \mathcal{P}^0(X_S^0)), \qquad +BC.
$$

$$
\begin{aligned}
\nabla^k_{p_1,j} u \quad & := (U^k_{p_1,j-1/2} - U^k_{p_1,j})\mu^k_{p_1,j|j-1/2} + (U^k_{p_1,j+1/2} - U^k_{p_1,j})\mu^k_{p_1,j|j+1/2}, \\
\widetilde{U}^k_{p_i,\sigma} \quad & = \mathbf{Coef}^k_{p_i} \widetilde{U}^k_{p_i}.
\end{aligned}
$$

Discrete spaces:

$$\begin{aligned}
\mathcal{V}_h^k &:= \left\{U^k : \Gamma_h^k \to \mathbb{R} \mid \forall\, S^k \subset \Gamma_h^k,\ U^k|_{S^k} = const\right\}\\
\mathcal{V}_{\partial\Gamma}^k &:= \left\{U_{\partial\Gamma}^k : \partial\Gamma_h^k \to \mathbb{R} \mid \forall\, p_i^k \in \partial\Gamma_h^k,\ U_{\partial\Gamma}^k|_{\sigma^k_{p_i,1/2}} = const,\ U_{\partial\Gamma}^k|_{\sigma^k_{p_i,n_{p_i}+1/2}} = const\right\}
\end{aligned}$$

Discrete norms:

$$\mathfrak{n}_S^k := \frac{1}{m_S^k} \sum_{p_i \in \partial S^k} \Big(m^k_{p_i,\mathcal{J}(p_i,S^k)-1/2} \mathcal{D}^k_{p_i,\mathcal{J}(p_i,S^k)} \nabla^k_{p_i,\mathcal{J}(p_i,S^k)} u \cdot n^k_{p_i,\mathcal{J}(p_i,S^k)|\mathcal{J}(p_i,S^k)-1/2} + m^k_{p_i,\mathcal{J}(p_i,S^k)+1/2} \mathcal{D}^k_{p_i,\mathcal{J}(p_i,S^k)} \nabla^k_{p_i,\mathcal{J}(p_i,S^k)} u \cdot n^k_{p_i,\mathcal{J}(p_i,S^k)|\mathcal{J}(p_i,S^k)+1/2}\Big)$$

O-Method Finite Volumes (Discretization)

Discrete spaces:

$$
\begin{aligned}
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\end{aligned}
$$

Discrete norms:

$$
\cap_S^k := \frac{1}{m_S^k} \sum_{p_i \in \partial S^k}
\Big(m^k_{p_i,\mathcal{J}(p_i,S^k)-1/2} \mathcal{D}^k_{p_i,\mathcal{J}(p_i,S^k)} \nabla^k_{p_i,\mathcal{J}(p_i,S^k)} u \cdot n^k_{p_i,\mathcal{J}(p_i,S^k)|\mathcal{J}(p_i,S^k)-1/2}
+ m^k_{p_i,\mathcal{J}(p_i,S^k)+1/2} \mathcal{D}^k_{p_i,\mathcal{J}(p_i,S^k)} \nabla^k_{p_i,\mathcal{J}(p_i,S^k)} u \cdot n^k_{p_i,\mathcal{J}(p_i,S^k)|\mathcal{J}(p_i,S^k)+1/2} \Big)
$$

$$
\begin{aligned}
-\textstyle\sum_{S^k} m_S^k\, U_S^k\, \cap_S^k &= \textstyle\sum_{p_i \in \Gamma_h^k} \left(\widetilde{U}^k_{p_i} \right)^\top A^k_{p_i}\, \widetilde{U}^k_{p_i} \\
&- \textstyle\sum_{p_i^k \in \partial\Gamma_h^k} \Big(m^k_{p_i,1/2}\, U^k_{p_i,1/2}\, \mathcal{D}^k_{p_i,1} \nabla^k_{p_i,1} u \cdot n^k_{p_i,1|1/2} \\
&+ m^k_{p_i,n_{p_i}+1/2}\, U^k_{p_i,n_{p_i}+1/2}\, \mathcal{D}^k_{p_i,n_{p_i}} \nabla^k_{p_i,n_{p_i}} u \cdot n^k_{p_i,n_{p_i}|n_{p_i}+1/2} \Big),
\end{aligned}
$$

where $A^k_{p_i}$ is a square matrix and $A^k_{p_i} \mathbf{1}_{p_i} = 0 \cdot \mathbf{1}_{p_i}$ $(\mathbf{1}_{p_i} := (1, 1, \cdots)^\top)$

Discrete norms:

$$
\begin{aligned}
&-\sum_{S^k} m_S^k\, U_S^k\, \cap_S^k = \sum_{p_i \in \Gamma_h^k} \left(\widetilde{U}_{p_i}^k\right)^\top A_{p_i}^k\, \widetilde{U}_{p_i}^k \\
&- \sum_{p_i^k \in \partial\Gamma_h^k} \Big(m_{p_i,1/2}^k\, U_{p_i,1/2}^k\, \mathcal{D}_{p_i,1}^k\, \nabla_{p_i,1}^k u \cdot n_{p_i,1|1/2}^k \\
&+ m_{p_i,n_{p_i}+1/2}^k\, U_{p_i,n_{p_i}+1/2}^k\, \mathcal{D}_{p_i,n_{p_i}}^k\, \nabla_{p_i,n_{p_i}}^k u \cdot n_{p_i,n_{p_i}|n_{p_i}+1/2}^k \Big),
\end{aligned}
$$

where $A_{p_i}^k$ is a square matrix and $A_{p_i}^k \mathbf{1}_{p_i} = 0 \cdot \mathbf{1}_{p_i}$ ($\mathbf{1}_{p_i} := (1, 1, \cdots)^\top$)

Remark:

$A_{p_i}^k$ depends only on $X_{p_i,j+1/2}^k$.

Discrete norms:

$$
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-&\textstyle\sum_{S^k} m_S^k\, U_S^k\, \cap_S^k = \sum_{p_i \in \Gamma_h^k} \left(\widetilde{U}_{p_i}^k\right)^\top A_{p_i}^k\, \widetilde{U}_{p_i}^k \\
&- \textstyle\sum_{p_i^k \in \partial\Gamma_h^k} \Big(m_{p_i,1/2}^k\, U_{p_i,1/2}^k\, \mathcal{D}_{p_i,1}^k \nabla_{p_i,1}^k u \cdot n_{p_i,1|1/2}^k \\
&+ m_{p_i,n_{p_i}+1/2}^k\, U_{p_i,n_{p_i}+1/2}^k\, \mathcal{D}_{p_i,n_{p_i}}^k \nabla_{p_i,n_{p_i}}^k u \cdot n_{p_i,n_{p_i}|n_{p_i}+1/2}^k \Big),
\end{aligned}
$$

where $A_{p_i}^k$ is a square matrix and $A_{p_i}^k \mathbf{1}_{p_i} = 0 \cdot \mathbf{1}_{p_i}$ $(\mathbf{1}_{p_i} := (1, 1, \cdots)^\top)$

Remark:

$A_{p_i}^k$ depends only on $X_{p_i,j+1/2}^k$.

Choose $X_{p_i,j+1/2}^k$ such that $A_{p_i}^k + (\mathbf{1}_{p_i} \otimes \mathbf{1}_{p_i})/n_{p_i}$ is strictly elliptic

Assumption: Any interior vertex p_i^k is surrounded by at least 3 cells.

Discrete norms:

$$-\sum_{S^k} m_S^k\, U_S^k\, \cap_S^k = \sum_{p_i \in \Gamma_h^k} \left(\widetilde{U}_{p_i}^k\right)^\top A_{p_i}^k\, \widetilde{U}_{p_i}^k$$
$$-\sum_{p_i^k \in \partial\Gamma_h^k} \Big(m_{p_i,1/2}^k\, U_{p_i,1/2}^k\, \mathcal{D}_{p_i,1}^k \nabla_{p_i,1}^k u \cdot n_{p_i,1|1/2}^k$$
$$+\, m_{p_i,n_{p_i}+1/2}^k\, U_{p_i,n_{p_i}+1/2}^k\, \mathcal{D}_{p_i,n_{p_i}}^k \nabla_{p_i,n_{p_i}}^k u \cdot n_{p_i,n_{p_i}|n_{p_i}+1/2}^k \Big),$$

where $A_{p_i}^k$ is a square matrix and $A_{p_i}^k \mathbf{1}_{p_i} = 0 \cdot \mathbf{1}_{p_i}$ $(\mathbf{1}_{p_i} := (1, 1, \cdots)^\top)$

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Discrete H_0^1 semi-norm: $\|U^k\|_{1,\Gamma_h^k}^2 := \sum_{p_i} \left(\widetilde{U}_{p_i}^k\right)^\top A_{p_i}^k \widetilde{U}_{p_i}^k$

Discrete $\mathbb{L}^2$ norm: $\|U^k\|_{\mathbb{L}^2(\Gamma_h^k)}^2 := \sum_S m_S^k \left(U_S^k\right)^2$

Theorem: The above discrete problem has a unique solution.

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Assume smooth variation of discrete points (The mesh does not stretch too much between two time steps). The stretch is bounded by $Ch\tau$.

Proposition 1: Stability, $\mathbb{L}^\infty(\mathbb{L}^2)$ and $\mathbb{L}^2(\mathbb{H}^1_0)$

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Proposition 1: Stability, $\mathbb{L}^\infty(\mathbb{L}^2)$ and $\mathbb{L}^2(\mathbb{H}_0^1)$

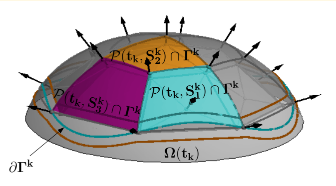
Assume smooth variation of discrete points (The mesh does not stretch too much between two time steps). The stretch is bounded by $Ch\tau$ and $A_{p_i}^k$ symmetric $\forall\, p_i^k$.

Proposition 2: Stability, $\mathbb{L}^2(\mathbb{L}^2)$ for $\partial_\tau U = \frac{U^{k+1} - U^k}{\tau}$, $\mathbb{L}^\infty(\mathbb{H}_0^1)$ for U

Theorem:
u: Real solution on $\Gamma(t)$,
U^k: Discrete solution on $\Gamma_h(t_k)$

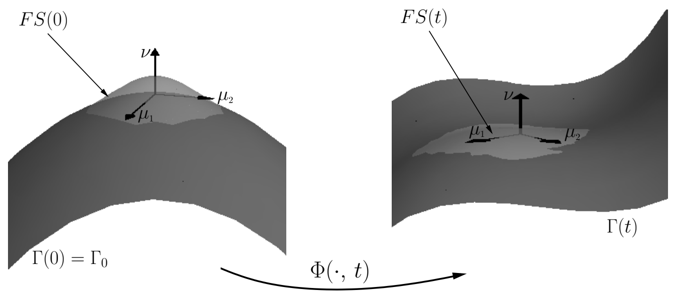
$$E^k = \sum_S \left(u^{-l}\left(X_S^k, t_k\right) - U_S^k\right)\chi_S$$

$\max_{1,\cdots,k_{max}} \|E^k\|^2_{\mathbb{L}^2(\Gamma_h^k)}$
$+\tau \sum_{k=1}^{k_{max}} \|E^k\|^2_{1,\Gamma_h^k} \leq C\,(h+\tau)^2$



$\mathcal{P}(\mathbf{x}(\mathbf{t_k}), \mathbf{t_k})$
$= \mathbf{x}(\mathbf{t_k}) - \mathbf{d}(\mathbf{x}(\mathbf{t_k}), \mathbf{\Omega}(\mathbf{t_k}))\nu(\mathcal{P}(\mathbf{x}(\mathbf{t_k}), \mathbf{t_k}))$
Extension of $\mathbf{u}$: $\nabla\mathbf{u}(\cdot, \mathbf{t_k}) \cdot \nabla\mathbf{d}(\cdot, \mathbf{\Gamma^k}) \equiv \mathbf{0}$,
$\mathbf{u}^{-\mathbf{l}}(\cdot, \mathbf{t_k}) := \mathbf{u}(\cdot, \mathbf{t_k})|_{\mathbf{\Gamma^k}}$

Modeling of surfactant driven thin film flow

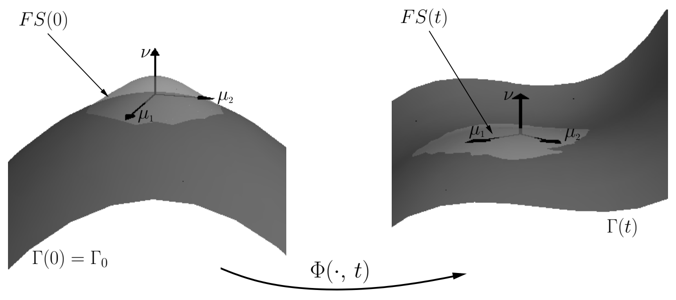


$\Gamma(t)$: Family of 2-d smooth surfaces

$\Phi(\cdot, t)$: Sufficiently smooth map, $\Phi(\Gamma(0), t) = \Gamma(t)$

$FS(t)$: Fluid Free Surface at t

Some variables:



$\Gamma(t)$: Family of 2-d smooth surfaces

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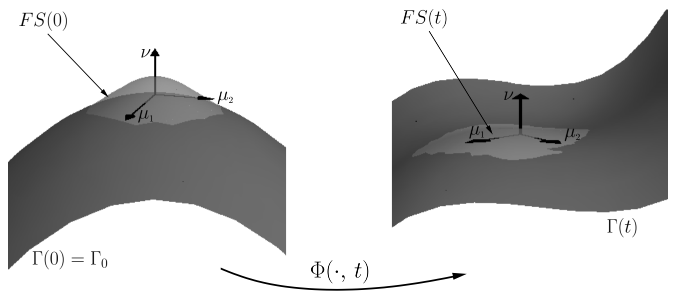
$FS(t)$: Fluid Free Surface at t

Some variables:

$\bar{\Pi}$: Surfactant concentration

$\bar{v}_{\mathcal{F}}$: velocity of the fluid particle, $\Phi(\Gamma(0), t) = \Gamma(t)$

$\bar{v}_{FS}$: velocity of the fluid particle on $FS(t)$



Surfactant equation

$$\begin{cases} \dfrac{\partial \bar{\Pi}}{\partial \bar{t}} + \left(\overline{\nabla}_{FS} \cdot \left(\bar{\Pi}\bar{v}_{FS}\right)\right) = \overline{\nabla}_{FS} \cdot (\bar{D}_{FS}\overline{\nabla}_{FS}\bar{\Pi}) \text{ on } FS \quad \text{(Stone 1990)} \\ (\bar{D}_{FS}\overline{\nabla}_{FS}\bar{\Pi}) \cdot n^{l}_{FS} = 0 \quad \text{on } \partial FS \end{cases}$$

Navier-Stokes equation

$$\begin{cases} \textbf{Mass conservation equation:} \quad \overline{\nabla} \cdot \bar{v}_{\mathcal{F}} = 0 \\ \textbf{Momentum equation:} \quad \mu\overline{\nabla} \cdot \left(\overline{\nabla}\bar{v}_{\mathcal{F}}\right) = \rho\dfrac{d\bar{v}_{\mathcal{F}}}{d\bar{t}} + \overline{\nabla}\bar{P} - \bar{f} \end{cases}$$

$+ \quad BC$

Thin film boundary condition

- No penetration on the substrate $\Gamma(t)$ $\Big((\bar{v}_{\mathcal{F}} - \bar{v}_{\Gamma}) \cdot \nu = 0\Big)$
- Slip boundary condition on the substrate $\Gamma(t)$ $\Big(\mu[\overline{T}_{\mathcal{F}}\nu]_{tan} = \bar{\beta}(\bar{v}_{\mathcal{F}} - \bar{v}_{\Gamma}), \quad (\overline{T}_{\mathcal{F}} = \overline{\nabla}\bar{v}_{\mathcal{F}} + (\overline{\nabla}\bar{v}_{\mathcal{F}})^{\top})\Big)$
- Kinematic boundary condition (Fluid particles remain on FS)
- Shear stress condition on FS: $\mu[\overline{T}_{\mathcal{F}}\nu_{FS}]_{FS,tan} = \overline{\nabla}_{FS}\bar{\gamma}$
- Laplace-Young boundary condition $\left[-\left(\bar{P} - \bar{P}_0\right)\nu_{FS} + \mu\overline{T}_{\mathcal{F}}\nu_{F,S}\right] \cdot \nu_{FS} = \bar{\gamma}\bar{\mathcal{K}}_{FS}$

μ : Viscosity

$\bar{\beta}$: Free surface tangential slip tensor

$\bar{P}_0$: Ambient pressure

ν_{FS} : Free surface normal

$\bar{\gamma}$: Surface tension

$\bar{P}$: Pressure

Equation of state

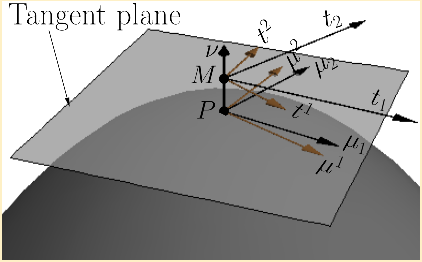
$$\bar{\gamma} = \bar{\gamma}_0 + R\,T_a\,\bar{\Pi}_\infty \ln(1 - \bar{\Pi}/\bar{\Pi}_\infty)$$

T_a : Absolute temperature (Kelvin)

R : Universal gas constant

$\bar{\gamma}_0$: Surface tension of the clean film $(\bar{\Pi}_0 = 0)$

$\bar{\Pi}_\infty$: Maximum possible surfactant concentration



Parameterization of $\Gamma(t)$: $\bar{X}(\bar{t}, \bar{s}), \quad \bar{s} = (\bar{s}_1, \bar{s}_2).$

Parameterization of the neighborhood of $\Gamma(t)$:
$\bar{r}(\bar{t}, \bar{s}, \bar{y}) = \bar{X}(\bar{t}, \bar{s}) + \bar{y}\nu(\bar{t}, \bar{s}).$

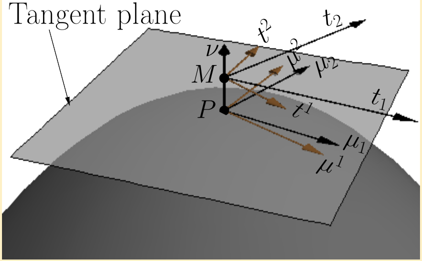
Curvilinear coordinate system:

Basis on $\Gamma(t)$:

$$\mu_1(\bar{t}, \bar{s}) = \frac{\partial \bar{X}(\bar{t}, \bar{s})}{\partial \bar{s}_1}$$
$$\mu_2(\bar{t}, \bar{s}) = \frac{\partial \bar{X}(\bar{t}, \bar{s})}{\partial \bar{s}_2}$$
$$\nu(\bar{t}, \bar{s}) = \frac{\mu_1(\bar{t}, \bar{s}) \wedge \mu_2(\bar{t}, \bar{s})}{\|\mu_1(\bar{t}, \bar{s}) \wedge \mu_2(\bar{t}, \bar{s})\|}$$

Basis in the neighborhood of $\Gamma(t)$:

$$t_1(\bar{t}, \bar{s}, \bar{y}) = \frac{\partial \bar{r}(\bar{t}, \bar{s}, \bar{y})}{\partial \bar{s}_1} = (\mathrm{Id} - \bar{y}\bar{K})\mu_1$$
$$t_2(\bar{t}, \bar{s}, \bar{y}) = \frac{\partial \bar{r}(\bar{t}, \bar{s}, \bar{y})}{\partial \bar{s}_2} = (\mathrm{Id} - \bar{y}\bar{K})\mu_2$$
$$t_3(\bar{t}, \bar{s}, \bar{y}) = \frac{\partial \bar{r}(\bar{t}, \bar{s}, \bar{y})}{\partial \bar{y}} = \nu(\bar{t}, \bar{s})$$



Scaling of variables: $\bar{s} = \mathcal{L}s, \quad \bar{y} = \mathcal{H}y, \quad \bar{t} = \mathcal{T}t, \quad \bar{K} = K/\mathcal{L},$

$$\bar{X}(\bar{t}, \bar{s}) = \mathcal{L}X(t, s), \quad \bar{r}(\bar{t}, \bar{s}) = \mathcal{L}r(t, s);$$

$$[r(t, s) = X(t, s) + \epsilon y \nu(t, s), \ (\epsilon = \mathcal{H}/\mathcal{L} << 1)]$$

Curvilinear coordinate system:

Basis on $\Gamma(t)$:

$$\mu_1(t, s) = \frac{\partial X(t,s)}{\partial s_1}$$

$$\mu_2(t, s) = \frac{\partial X(t,s)}{\partial s_2}$$

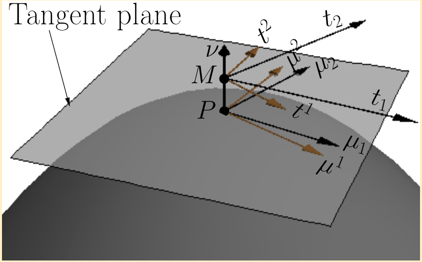
$$\nu(t, s) = \frac{\mu_1(t,s) \wedge \mu_2(t,s)}{\|\mu_1(t,s) \wedge \mu_2(t,s)\|}$$

Basis in the neighborhood of $\Gamma(t)$:

$$t_1(t, s, y) = \frac{\partial r(t,s,y)}{\partial s_1} = (\mathrm{Id} - \epsilon y K)\mu_1$$

$$t_2(t, s, y) = \frac{\partial r(t,s,y)}{\partial s_2} = (\mathrm{Id} - \epsilon y K)\mu_2$$

$$t_3(t, s, y) = \frac{\partial r(t,s,y)}{\partial y} = \epsilon \nu(t, s)$$



Decomposition of the velocity:

Fluid particle at M**:** $r(t, s_1(t), s_2(t), y(t))$

$$v_{\mathcal{F}} = \frac{dr}{dt} = (v_\Gamma + v_{R,tan}) + \epsilon(v_{mF} + v_{R,\nu}\nu), \quad \text{with}$$

$$v_\Gamma = \frac{\partial X}{\partial t}, \qquad v_{R,tan} = (\,\mathrm{Id} - \epsilon y K)\left(\frac{\partial s_1}{\partial t}\mu_1 + \frac{\partial s_2}{\partial t}\mu_2\right),$$

$$v_{R,\nu} = \frac{dy}{dt}, \qquad v_{mF} = -y\left(\nabla_\Gamma\left(v_\Gamma \cdot \nu\right) + K v_\Gamma\right).$$

Height of the film: $\mathtt{H}$

Surfactant equation:

$$\begin{cases} \dfrac{\partial \Pi}{\partial t} + (\nabla_{FS} \cdot (\Pi v_{FS})) = & \dfrac{1}{\mathcal{P}_e} \nabla_{FS} \cdot (D_{FS} \nabla_{FS} \Pi) \qquad \text{on } FS, \\ (D_{FS} \nabla_{FS} \Pi) \cdot n^l_{FS} = & 0 \qquad \text{on } \partial FS. \end{cases}$$

Momentum equation projected on axis approximated at ϵ^2 order:

$$\begin{cases} \dfrac{\partial P}{\partial y} = & \epsilon \mathcal{B}_0 f_\nu \\ -\epsilon \mathcal{K} \dfrac{\partial v_{R,tan}}{\partial y} + \dfrac{\partial^2 v_{R,tan}}{\partial y^2} = & \nabla_\Gamma P + \epsilon y K \nabla_\Gamma P - \mathcal{B}_0 f_{tan} \end{cases}$$

Boundary condition approximated at ϵ^2 order:

No penetration on Γ : $\quad v_{R,\nu} = 0$

Friction slip condition on Γ : $\quad \dfrac{\partial v_{R,tan}}{\partial y} + \epsilon K v_{R,tan} = \beta v_{R,tan}$

Shear stress condition on FS : $\quad \dfrac{\partial v_{R,tan}}{\partial y} + \epsilon K v_{R,tan} = \left(\mathrm{Id} + \epsilon \mathsf{H} K\right) \nabla_\Gamma \gamma$

Laplace-Young's law on FS : $\quad P = P_0 - C' \gamma \mathcal{K}_{FS},$

Algorithm for the derivation of the reduced model of the thin-film equation

1. Momentum equation projected on axis approximated at ϵ^2 order:

$$\int_y^{\mathtt{H}} \frac{\partial P}{\partial y} dy = \int_y^{\mathtt{H}} \epsilon \mathcal{B}_0 f_\nu dy \implies P(y) = P_0 - C' \gamma \mathcal{K}_{FS} + \epsilon \mathcal{B}_0 f_\nu (y - \mathtt{H})$$

2. **Set** $v_{R,tan} = v_0 + y v_1 + y^2 v_2 + y^3 v_3 + y^4 v_4 + y^5 v_5 + \cdots$ and integrate

$$\int_0^y -\epsilon \mathcal{K} \frac{\partial v_{R,tan}}{\partial y} + \frac{\partial^2 v_{R,tan}}{\partial y^2} dy = \int_0^y \nabla_\Gamma P + \epsilon y K \nabla_\Gamma P - \mathcal{B}_0 f_{tan} dy$$

at $\mathcal{O}(\epsilon^2)$ order using power series.

3. Multiply the mass conservation equation by

$$dS_{\Gamma,var} = \left[(t_1 \wedge t_2) \cdot \nu\right] \left[(\mu_1 \wedge \mu_2) \cdot \nu\right]^{-1} = 1 - \epsilon y \mathcal{K} + \frac{1}{2} \epsilon^2 y^2 (\mathcal{K}^2 - \mathcal{K}_2)$$

and integrate the result along ν from 0 to $\mathtt{H}$.

$$\frac{\partial^\Gamma \eta}{\partial t} + \eta \nabla_\Gamma \cdot v_\Gamma + \nabla_\Gamma \cdot F dy = 0,$$

$$\eta = \int_0^{\mathtt{H}} dS_{\Gamma,var} dy = \mathtt{H} - \frac{1}{2}\epsilon \mathtt{H}^2 \mathcal{K} + \frac{1}{6}\epsilon^2 \mathtt{H}^3 \left(\mathcal{K}^2 - \mathcal{K}_2\right),$$

$$F = \int_0^{\mathtt{H}} \left[\left(\mathrm{Id} - \epsilon y \left(\mathcal{K}\,\mathrm{Id} - K\right)\right) v_{R,tan}\right] dy.$$

Simulation of surfactant driven thin film flow

Thin-Film equation:

$$\frac{\partial^\Gamma \eta}{\partial t} + \eta \nabla_\Gamma \cdot v_\Gamma + \nabla_\Gamma \cdot F dy = 0,$$

$$+ \; BC$$

Surfactant equation:

$$\begin{cases} \dfrac{\partial \Pi}{\partial t} + (\nabla_{FS} \cdot (\Pi v_{FS})) = & \dfrac{1}{\mathcal{P}_e} \nabla_{FS} \cdot (D_{FS} \nabla_{FS} \Pi) \qquad \text{on } FS, \\ (D_{FS} \nabla_{FS} \Pi) \cdot n^l_{FS} = & 0 \qquad \text{on } \partial FS. \end{cases}$$

Equation of state:

$$\gamma = \frac{1 + E \ln(1 - x\Pi)}{1 + E \ln(1 - x)}.$$

Surfactant driven thin film equation

$$\begin{cases} \mathfrak{P} \;=\; -\epsilon \Delta_{\Gamma} \mathsf{H} \\ \dfrac{\partial \eta}{\partial t} + \eta \nabla_{\Gamma} \cdot v_{\Gamma} + \nabla_{\Gamma} \cdot [-\mathfrak{D}_1 \nabla_{\Gamma} (\phi + C' \gamma \mathfrak{P}) + \mathfrak{D}_2 \nabla_{\Gamma} \gamma + \mathfrak{D}_7 \nabla_{\Gamma} \mathsf{H}] \\ + \sum_j \nabla_{\Gamma} \cdot (\mathfrak{D}_j \nabla_{\Gamma} \omega_j) \;=\; 0 \\ \dfrac{\partial \Pi}{\partial t} + \Pi \nabla_{FS} \cdot v_{p\nu} \\ + \nabla_{FS} \cdot (\mathfrak{D}_{FS,1} \nabla_{\Gamma} (\phi + C' \gamma \mathfrak{P}) + \mathfrak{D}_{FS,2} \nabla_{\Gamma} \gamma + \mathfrak{D}_{FS,3} \nabla_{\Gamma} \mathsf{H}) \\ + \sum_j \nabla_{FS} \cdot (\mathfrak{D}_{FS,j} \nabla_{\Gamma} \omega_j) \;-\; \dfrac{1}{\mathcal{P}_e} \nabla_{FS} \cdot (D_{FS} \nabla_{FS} \Pi) \;=\; 0. \end{cases}$$

$v_{p\nu}$: velocity of the free surface particle parallel to ν.
$\mathfrak{D}_j = \mathfrak{D}_j(\mathsf{H}, K, g_\nu)$: substrate tensor.
$\mathfrak{D}_{FS,j} = \mathfrak{D}_{FS,j}(\mathsf{H}, K, g_\nu)$: Free surface tensor.
$\omega_j := \mathcal{K}, \mathcal{K}_2, g_{tan}$.

Surfactant driven thin film equation

$$
\left\{
\begin{aligned}
&\mathfrak{P} \;=\; -\epsilon \Delta_{\Gamma} \mathsf{H} && (1)\\
&\frac{\partial \eta}{\partial t} + \eta \nabla_{\Gamma} \cdot v_{\Gamma} + \nabla_{\Gamma} \cdot \left[-\mathfrak{D}_1 \nabla_{\Gamma} \left(\phi + C' \gamma \mathfrak{P} \right) + \mathfrak{D}_2 \nabla_{\Gamma} \gamma + \mathfrak{D}_7 \nabla_{\Gamma} \mathsf{H} \right] \\
&+ \sum_j \nabla_{\Gamma} \cdot \left(\mathfrak{D}_j \nabla_{\Gamma} \omega_j \right) \;=\; 0 && (2)\\
&\frac{\partial \Pi}{\partial t} + \Pi \nabla_{FS} \cdot v_{p\nu} \\
&+ \nabla_{FS} \cdot \left(\mathfrak{D}_{FS,1} \nabla_{\Gamma} \left(\phi + C' \gamma \mathfrak{P} \right) + \mathfrak{D}_{FS,2} \nabla_{\Gamma} \gamma + \mathfrak{D}_{FS,3} \nabla_{\Gamma} \mathsf{H} \right) \\
&+ \sum_j \nabla_{FS} \cdot \left(\mathfrak{D}_{FS,j} \nabla_{\Gamma} \omega_j \right) \;-\; \frac{1}{\mathcal{P}_e} \nabla_{FS} \cdot \left(D_{FS} \nabla_{FS} \Pi \right) \;=\; 0. && (3)
\end{aligned}
\right.
$$

$$
\left\{
\begin{aligned}
&(\nabla_{\Gamma} \mathsf{H}) \cdot n^l_{\partial \Gamma} \;=\; 0 && \text{on } \partial \Gamma && (4)\\
&\left[-\mathfrak{D}_5 \nabla_{\Gamma} (\Phi + C' \gamma \mathfrak{P}) \right] \cdot n^l_{\partial \Gamma} \;=\; 0 && \text{on } \partial \Gamma && (5)\\
&(D_{FS} \nabla_{FS} \Pi) \cdot n^l_{FS} = 0 && \text{on } \partial FS. && (6)
\end{aligned}
\right.
$$

Algorithm:

- For each cell S, construct a local orthonormal basis $(e^k_{S,1}, e^k_{S,2}, \nu_S)$
- Use the gradients of u obtained on subcells using Id, to construct a minmod gradient $\nabla^k_S u$ on the cell S
- Construct the fluxes produced by the operator $\nabla_\Gamma \cdot (\nabla_\Gamma Q)$ on subedges
- Apply the standard upwind methodology using the mid point on edges

Algorithm:

Projection onto the free surface in the direction of ν: $\mathbb{P}(\cdot, t)$

Curved mesh on the free surface: $\mathbb{P}(\Gamma_h^k, t_k)$

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Parameterization of the substrate $\Gamma(t)$: $X(s,t), \quad s = (s_1, s_2)$

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Unit normal to $FS(t)$: $\nu_{FS} = \frac{\nu - \epsilon R_{\mathsf{H}} \nabla_\Gamma \mathsf{H}}{\sqrt{1+\epsilon^2 \|R_{\mathsf{H}} \nabla_\Gamma \mathsf{H}\|^2}}, \qquad R_{\mathsf{H}} = (\,\mathrm{Id} - \epsilon \mathsf{H} K)^{-1}$

Important observation:

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Important observation:

μ tangent on $\Gamma(t) \quad \mapsto \quad (\,\mathrm{Id} - \epsilon \mathsf{H} K)\mu + \epsilon[(\nabla_\Gamma \mathsf{H}) \cdot \mu]\nu$ tangent on $FS(t)$

Approximations on free surface curved subcell $\mathbb{P}(S_{p_i,j}^k, t_k)$:

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Project the finite volume setup described on the substrate onto the free surface.

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Unit normal to $FS(t)$: $\nu_{FS} = \frac{\nu - \epsilon R_{\mathsf{H}} \nabla_\Gamma \mathsf{H}}{\sqrt{1+\epsilon^2 \| R_{\mathsf{H}} \nabla_\Gamma \mathsf{H} \|^2}}, \qquad R_{\mathsf{H}} = (\,\mathrm{Id} - \epsilon \mathsf{H} K)^{-1}$

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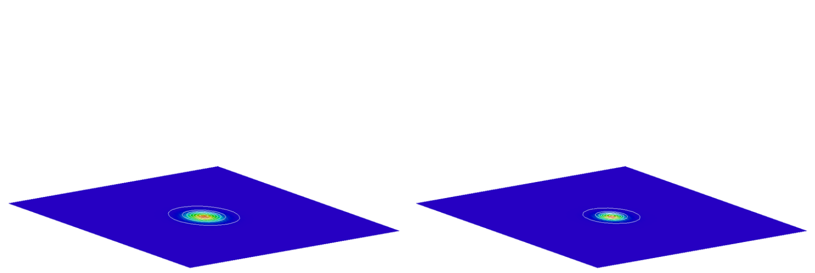
Approximations on free surface curved subcell $\mathbb{P}(S^k_{p_i,j}, t_k)$:

Project the finite volume setup described on the substrate onto the free surface.

The finite volume scheme follows the same path as described above (O-method finite volume).

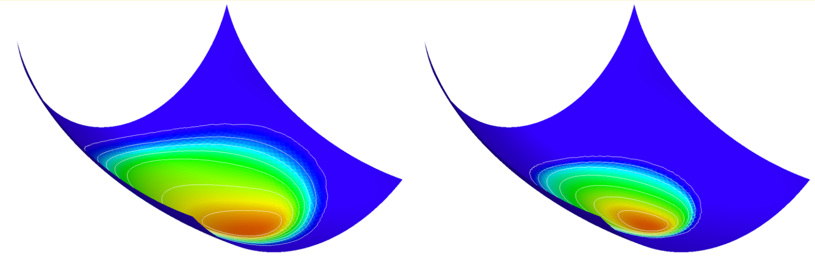
- Surfactant-Thin-film flowing on an evolving plane

Thin-film evolution ⇓ | Surfactant evolution ⇓



- Surfactant-Thin-film flowing on an evolving plane

Thin-film evolution ⇓ Surfactant evolution ⇓



Summary

- Robust Finite Volumes scheme for convection-diffusion reaction on polygonal surfaces
- Modeling of surfactant driven thin film flow
- Finite Volumes for PDE defined on moving free interfaces
- Fully coupled model for surfactant driven thin-film flow

Perspectives

- The technique is easily extended to tree dimension,
- One can also extend to higher order Finite volumes,
- The combination of this method with an appropriate mesh optimization tool will give a more stable scheme for skewed movement.

cf.:

1. Martin Lenz, Simplice Firmin Nemadjieu, and Martin Rumpf, *Finite Volume Method on Moving Surfaces*, Finite Volumes for Complex applications V, Wiley, 2008, p. 561–568.

2. Martin Lenz, Simplice Firmin Nemadjieu, and Martin Rumpf, *A Convergent Finite Volume Scheme for Diffusion on Evolving Surfaces*, SIAM J. Numer. Anal. 49, 2011, p. 15–37.

3. Simplice Firmin Nemadjieu, *A Convergent Finite Volume Type O-method on Evolving Surfaces*, AIP Conference Proceedings; 9/30/2010, Vol. 1281, Issue 1, p. 2184 –2187.

THANK YOU FOR YOUR ATTENTION

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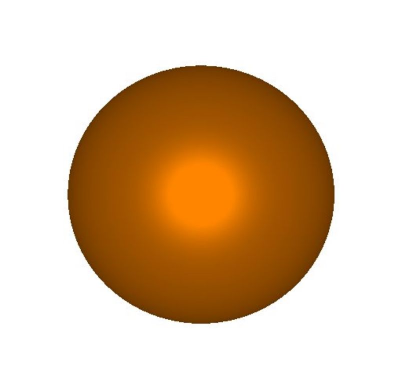
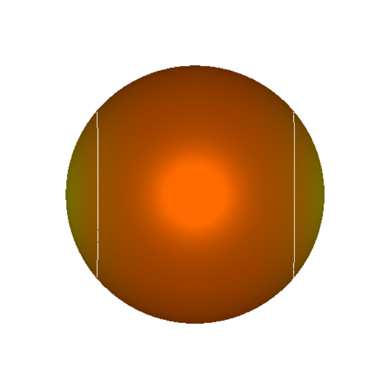
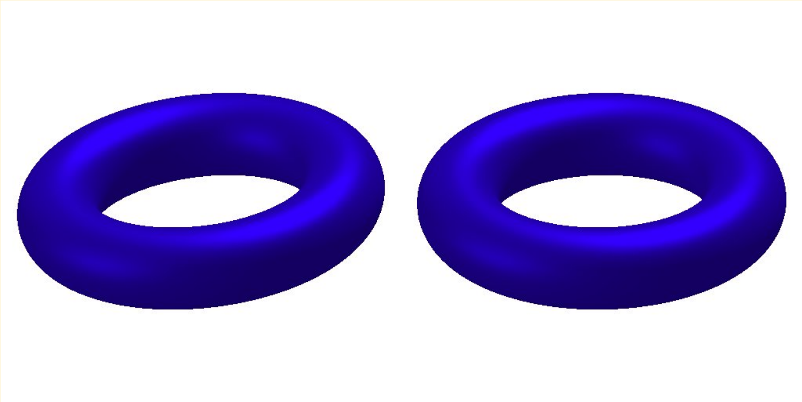


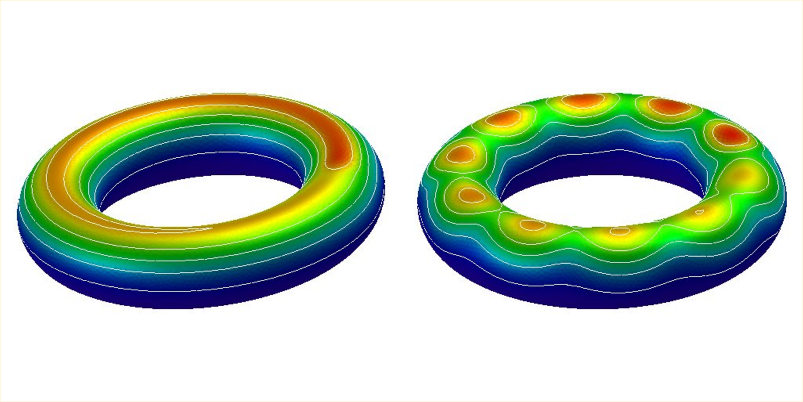


$\mathcal{D}_0 = Id$



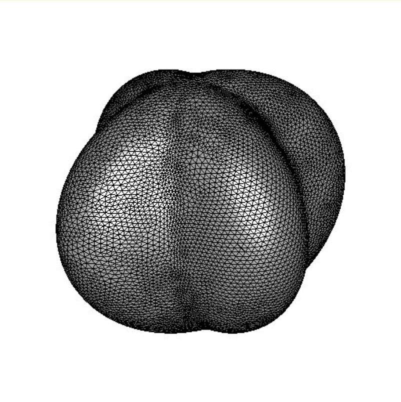
Time indepentent source term   Periodic source term

Numerical Results: Heat equation on rotative torus



Time indepentent source term   Periodic source term

Numerical Results: Advection-diffusion equation



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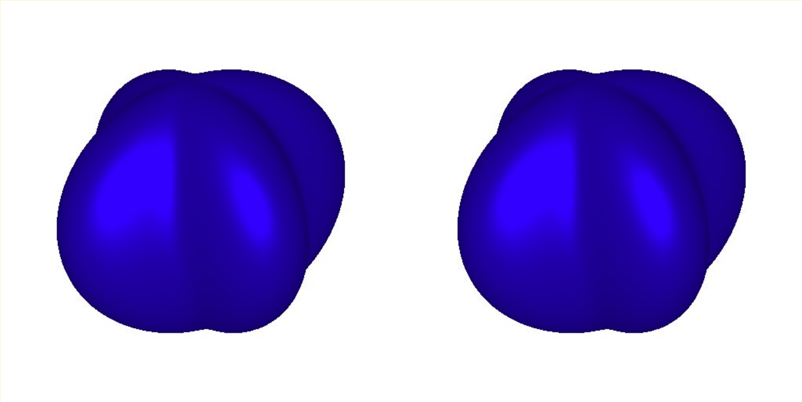

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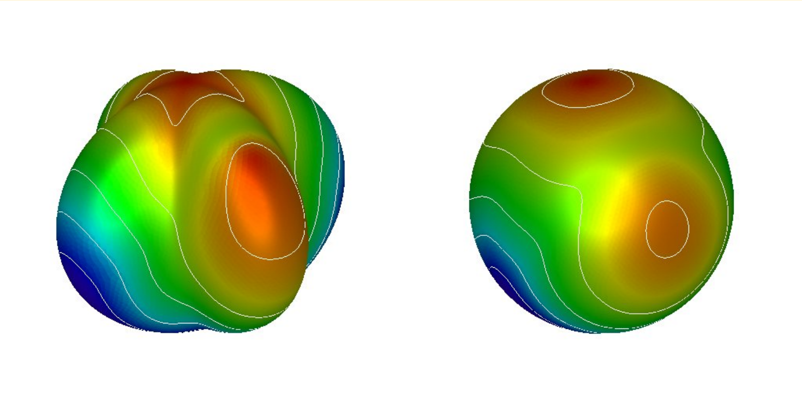
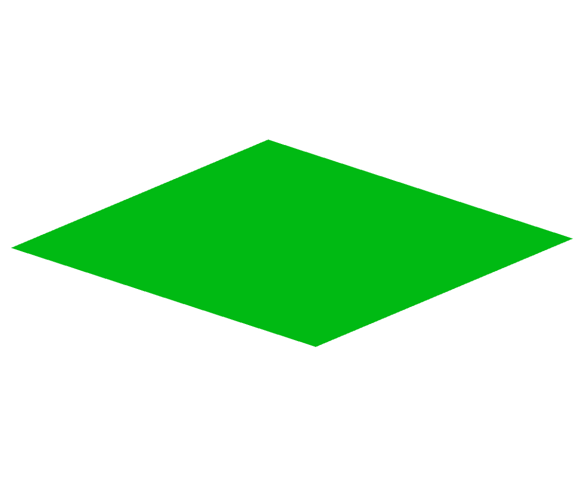


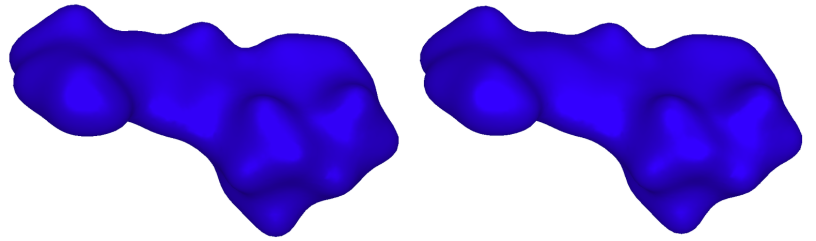
- Advection-Diffusion-Reaction on surfaces



- Advection-Diffusion-Reaction on surfaces

Evolution of surface by mean-curvature flow ⇓

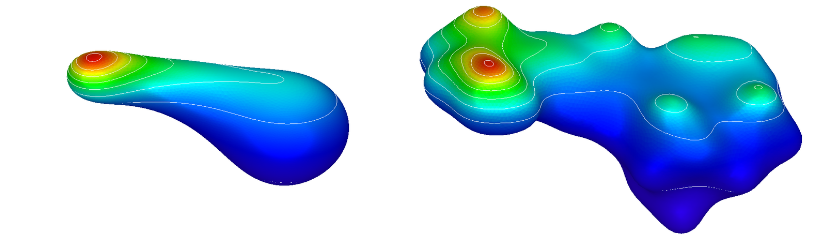
Static surface ⇓



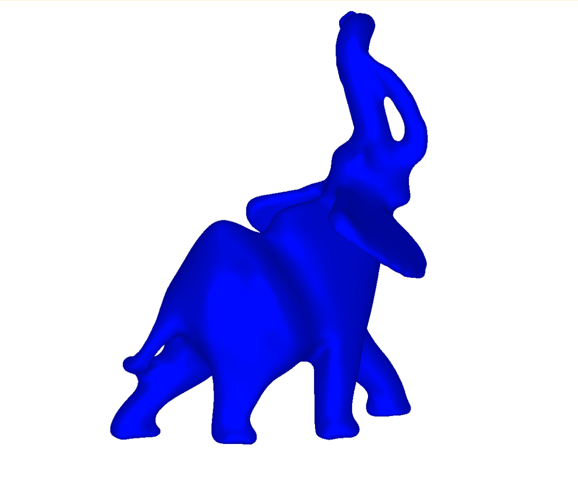
- Advection-Diffusion-Reaction on surfaces

Evolution of surface by mean-curvature flow ⇓

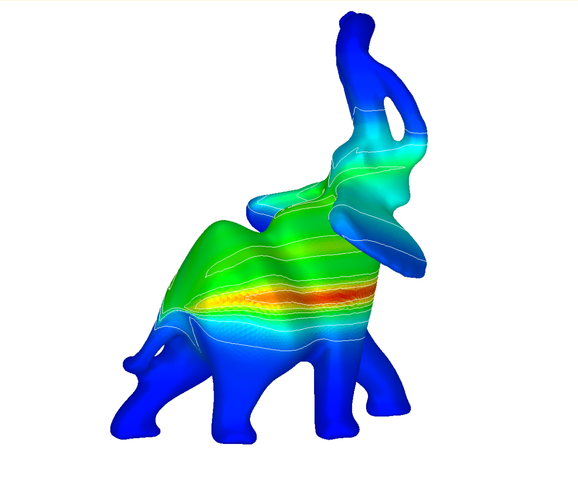
Static surface ⇓



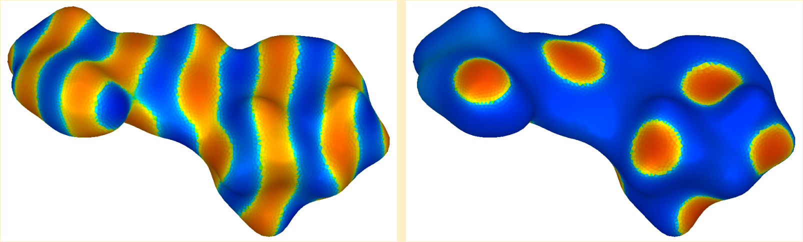
- Highly anisotropic Diffusion on surfaces



- Highly anisotropic Diffusion on surfaces



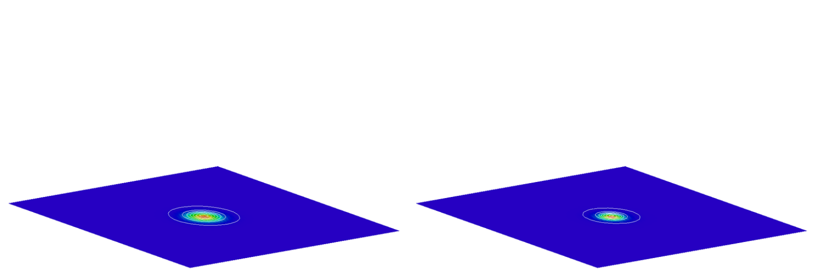
- Pattern formation on surfaces
- Textures generation on surfaces



Simulation of surfactant driven thin film flow (Numerical results)

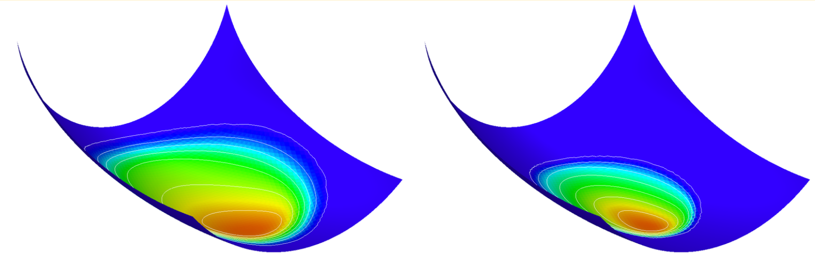
- Surfactant-Thin-film flowing on an evolving plane

Thin-film evolution $\Downarrow$ Surfactant evolution $\Downarrow$

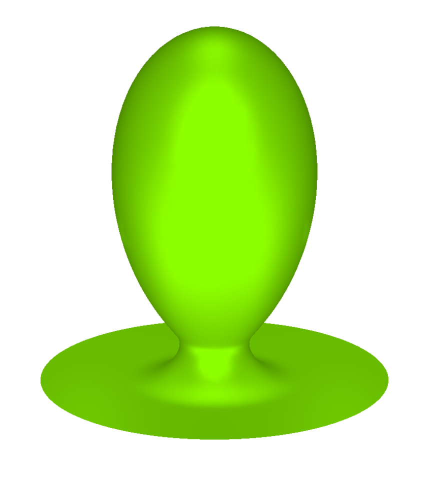


- Surfactant-Thin-film flowing on an evolving plane

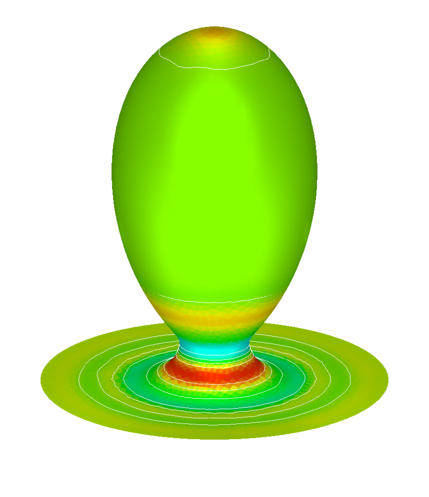
Thin-film evolution ⇓   Surfactant evolution ⇓



- Thin-film flow in a lung alveolus

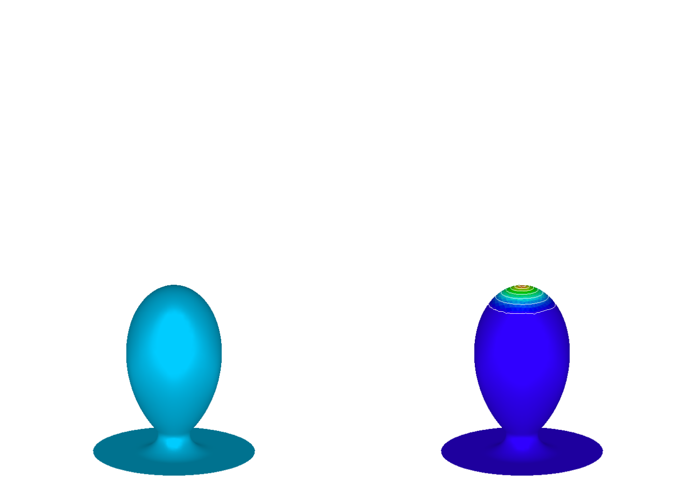


- Thin-film flow in a lung alveolus



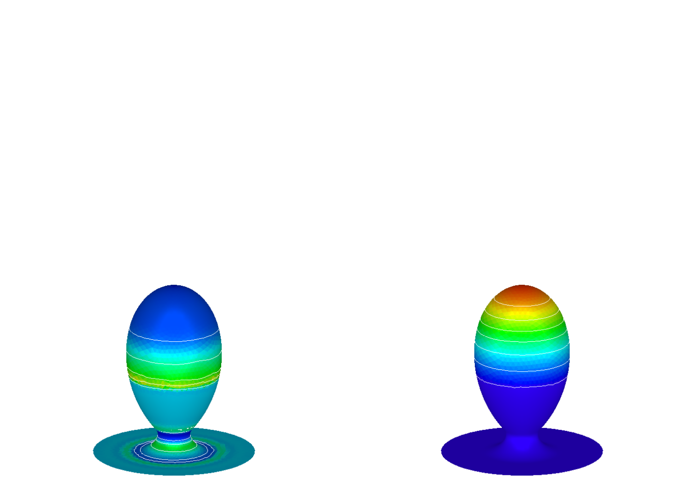
- Surfactant-Thin-film flowing in a lung alveolus

Thin-film evolution ⇓ Surfactant evolution ⇓



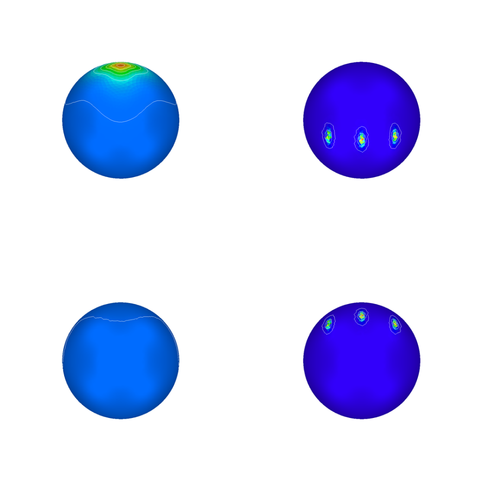
- Surfactant-Thin-film flowing in a lung alveolus

Thin-film evolution ⇓ Surfactant evolution ⇓



- Surfactant-Thin-film flowing on an evolving sphere

Thin-film evolution ⇓ Surfactant evolution ⇓

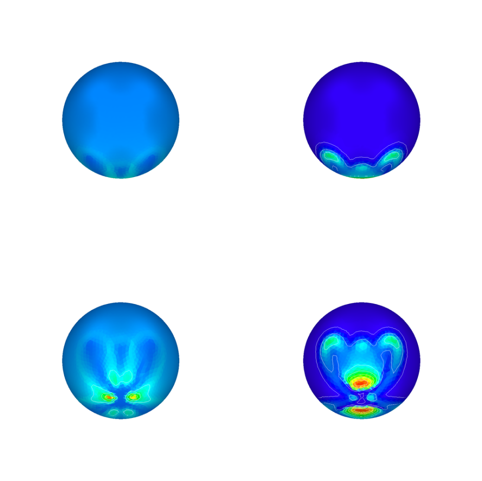


⟸ Seen 30^o from above

⟸ Seen 50^o from below

- Surfactant-Thin-film flowing on an evolving sphere

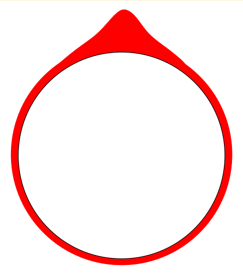
Thin-film evolution ⇓ Surfactant evolution ⇓



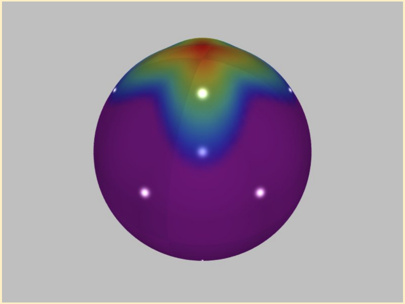
⟸ Seen 30^o from above

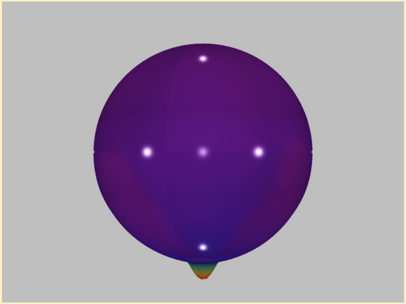
⟸ Seen 50^o from below

Numerical Results: Thin film on sphere (with gravity)



Numerical Results: Thin film on sphere (with gravity)





Numerical Results: Thin film on curved surface (without gravity)