Bulk-surface multiphysics coupling

A CutFEM approach with boundary conditions à la Nitsche

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Model problem

Bulk-interface scalar equations

Interaction between the surface and the bulk.

$$
\begin{aligned}
-\nabla \cdot (k_B \nabla u_B) &= f_B && \text{in } \Omega, \\
-\boldsymbol{n} \cdot k_B \nabla u_B &= b_B u_B - b_S u_S && \text{on } \Gamma, \\
-\nabla_\Gamma \cdot (k_S \nabla_\Gamma u_S) &= f_S - \boldsymbol{n} \cdot k_B \nabla u_B && \text{on } \Gamma.
\end{aligned}
$$

Physics: concentration of surfactants interacting with a bulk concentration, proton transport via a membrane surface, etc.

Math: coupling between a Poisson's equation and a Laplace-Beltrami equation.

`deal.II` implementation idea

Implementation through an **iterative method**.

- Initial guess for the bulk solution;
- solve the surface problem: `LaplaceBeltramiProblem`;
- solve the bulk problem: `CutFEMSolver`;
- iteratively solve surface and bulk problems up to convergence.

The Laplace-Beltrami operator

Tangential gradient

- Parametrized surfaces:

$$(\nabla_\Gamma f)\,(X(\boldsymbol{\theta})) = \sum_{i,j=1}^{n} \mathrm{G}_{ij}^{-1}(\boldsymbol{\theta})\,\frac{\partial F}{\partial \theta_j}(\boldsymbol{\theta})\,\frac{\partial X}{\partial \theta_i}(\boldsymbol{\theta}),$$

  where

$$F(\boldsymbol{\theta}) = f(X(\boldsymbol{\theta})), \qquad \mathrm{G} = \frac{\partial X}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta})\,\frac{\partial X}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}).$$

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- Hypersurfaces:

$$\nabla_\Gamma f(x) = \nabla \tilde{f}(x) - \left(\nabla \tilde{f}(x) \cdot \boldsymbol{n}\right) \boldsymbol{n} = (\mathrm{I} - \boldsymbol{n} \otimes \boldsymbol{n}) \nabla \tilde{f}(x).$$

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Locally, we can use both definitions!

Laplace-Beltrami operator

Then, the Laplace-Beltrami operator is

$$\Delta_\Gamma f = \nabla_\Gamma \cdot \nabla_\Gamma f.$$

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No boundaries $\implies$ generalization of the Green's formula:

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Thus, integrals can be approximated as

$$\int_K \nabla_\Gamma f \cdot \nabla_\Gamma v \approx \sum_{q=1}^{N_q} (\nabla(f(X))(x_q))^T \mathrm{G}^{-1}(x_q) \nabla(v(X))(x_q) \sqrt{\det(\mathrm{G}(x_q))}\, w_q$$

`class LaplaceBeltramiProblem`

Main features of the `class`:

- geometry dependent on
  - embedding space dimension **`spacedim`**;
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- the code **automatically** deals with **codimension one** object
  - `FEValues::shape_grad(j,q)` $\Longrightarrow$ $\nabla X_K(x_q)\, G^{-1}(x_q) \nabla(\varphi_j(X_K))$;
  - `FEValues::JxW(q)` $\Longrightarrow$ $\sqrt{\det(G^{-1}(x_q))}\, w_q$;

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- `GridGenerator::extract_boundary_mesh`:
  from volume to surface mesh.

Well-posedness of the model

Weak formulation

- Bulk equation: $w_B \in H^1(\Omega)$

$$(k_B \nabla u_B, \nabla w_B)_\Omega + (b_B u_B - b_S u_S, w_B)_\Gamma = (f_B, w_B)_\Omega \quad \forall\, w_B \in H^1(\Omega)\,.$$

- Surface equation: $w_S \in H^1(\Gamma)$

$$(k_S \nabla_\Gamma u_S, \nabla_\Gamma w_S)_\Gamma - (b_B u_B - b_S u_S, w_S)_\Gamma = (f_S, w_S)_\Gamma \quad \forall\, w_S \in H^1(\Gamma)\,.$$

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No unique solution: additional constraint required.

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No unique solution: additional constraint required.

$$\int_\Gamma u_S = 0 \implies \text{uniqueness!}$$

Weak formulation

Find $(u_B, u_S) \in V = V_B \times V_S = H^1(\Omega) \times \left(H^1(\Gamma)/\langle \mathcal{C}_\Gamma \rangle\right)$ such that

$$\mathcal{A}\left((u_B, u_S), (v_B, v_S)\right) = \mathcal{F}\left((v_B, v_S)\right) \qquad \forall\, (v_B, v_S) \in V.$$

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- Bilinear form:

$$\begin{aligned} \mathcal{A}\left((u_B, u_S), (v_B, v_S)\right) &= b_B\left(k_B \nabla u_B, \nabla v_B\right)_\Omega && (1)\\ &+ b_S\left(k_S \nabla_\Gamma u_S, \nabla_\Gamma v_S\right)_\Gamma && (2)\\ &+ \left(b_B u_B - b_S u_S, b_B v_B - b_S v_S\right)_\Gamma . && (3) \end{aligned}$$

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\end{aligned}$$

- Linear functional:

$$\mathcal{F}\left((v_B, v_S)\right) = b_B\left(f_B, v_B\right)_\Omega + b_S\left(f_S, v_S\right)_\Gamma .$$

Continuity of $\mathcal{A}$

V-norm: $\|(v_B, v_S)\|_V = \left(\|u_B\|_{V_B}^2 + \|u_S\|_{V_S}^2\right)^{1/2}$.

We subdivide the computation into two:

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\begin{aligned}
(1) + (2) &\leq \max\{b_B k_B,\, b_S k_S\}\left(\|u_B\|_{V_B}\|v_B\|_{V_B} + \|u_S\|_{V_S}\|v_S\|_{V_S}\right)\\
&\leq \sqrt{2}\max\{b_B k_B,\, b_S k_S\}\left(\|u_B\|_{V_B}^2 + \|u_S\|_{V_S}^2\right)^{1/2}\left(\|v_B\|_{V_B}^2 + \|v_S\|_{V_S}^2\right)^{1/2}\\
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\end{aligned}
$$

$$
\begin{aligned}
(3) &\leq \max\{b_B,\, b_S\}^2 \left(\|u_B\|_{L^2(\Gamma)} + \|u_S\|_{L^2(\Gamma)} \right) \left(\|v_B\|_{L^2(\Gamma)} + \|v_S\|_{L^2(\Gamma)} \right) \\
&\leq c_T^2 \max\{b_B,\, b_S\}^2 \left(\|u_B\|_{V_B} + \|u_S\|_{V_S} \right) \left(\|v_B\|_{V_B} + \|v_S\|_{V_S} \right) \\
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$\mathcal{A}(\cdot,\cdot)$ is continuous.

Coercivity of $\mathcal{A}$ and continuity of $\mathcal{F}$

Thanks to the Poincaré-Wirtinger inequality

$$\begin{aligned}
\mathcal{A}\left(\left(u_B, u_S\right), \left(u_B, u_S\right)\right) &\geq b_B k_B \|\nabla u_B\|^2_{L^2(\Omega)} + b_S k_S \|\nabla u_S\|^2_{L^2(\Gamma)} \\
&\geq \frac{b_B k_B}{c^2_{P,B} + 1} \|u_B\|^2_{V_B} + \frac{b_S k_S}{c^2_{P,S} + 1} \|u_S\|^2_{V_S} \\
&\geq \alpha \| \left(u_B, u_S\right) \|^2_V
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Then,

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Then,

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$$

$\mathcal{F}(\cdot)$ is continuous.

The Cut Finite Element Method

An immersed method

The mesh is unfitted to the domain Ω, defined through a level set function ψ.

$$\Omega = \{x \in \mathbb{R}^2 : \psi(x) < 0\},$$
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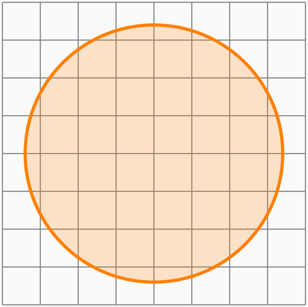

(a) Background mesh

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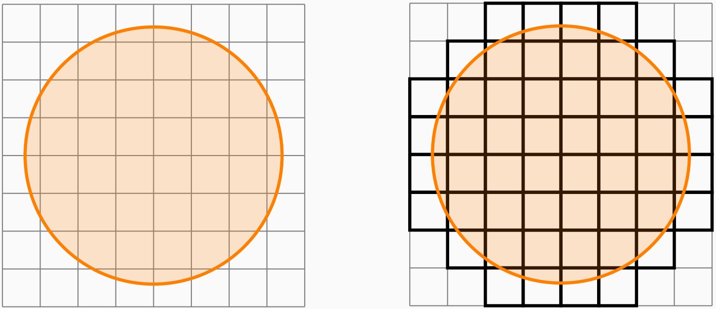

(a) Background mesh (b) Active mesh

Boundary conditions with Nitsche's method

Boundary conditions imposed **weakly** through the **Nitsche's method.**

$$-\Delta u = f \quad \text{in } \Omega, \qquad\qquad \varepsilon \frac{\partial u}{\partial \boldsymbol{n}} + u = g \quad \text{on } \Gamma.$$

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Then, the (bi-)linear forms for the Nitsche's method are

$$\begin{aligned}\mathcal{B}_h(u, v) = (\nabla u, \nabla v)_\Omega + \sum_{F \in \mathcal{G}_h} \Bigg\{ &- \frac{\gamma h_F}{\varepsilon + \gamma h_F} \left[\left(\frac{\partial u}{\partial \boldsymbol{n}}, v \right)_F + \left(u, \frac{\partial v}{\partial \boldsymbol{n}} \right)_F \right] \\ &+ \frac{1}{\varepsilon + \gamma h_F} (u, v)_F - \frac{\varepsilon \gamma h_F}{\varepsilon + \gamma h_F} \left(\frac{\partial u}{\partial \boldsymbol{n}}, \frac{\partial v}{\partial \boldsymbol{n}} \right)_F \Bigg\},\end{aligned}$$

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Remark: loss of coercivity when $\varepsilon \to 0$ for every value of γ!

Ghost penalty stabilization

We add a penalization term of the form

$$j_h(u_h, v_h) = \gamma_A \sum_{F \in \mathscr{F}_h} \left(h_F \left[\frac{\partial u_h}{\partial \boldsymbol{n}} \right], \left[\frac{\partial v_h}{\partial \boldsymbol{n}} \right] \right)_F .$$

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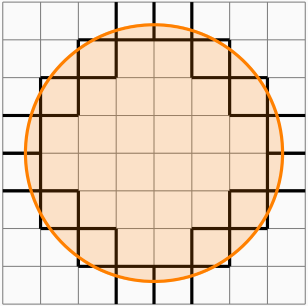

Figure 2: Faces with ghost penalty

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- `hp::FECollection`
  - **`FE_Q`** for `inside` and `intersected` cells;
  - **`FE_Nothing`** for `outside` cells;
- `NonMatching::FEValues`: quadrature rules for `inside` and `intersected` cells.

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- coupling between bulk and surface in a scalar problem;
- `dim-spacedim` compatible version of `point_value()`;
- increments-based iterative method
  - $\|u_B^{(k+1)} - u_B^{(k)}\|_{L^2(\Omega)} < \mathtt{tol}$;
  - $\|u_S^{(k+1)} - u_S^{(k)}\|_{L^2(\Gamma)} < \mathtt{tol}$.

Results

Numerical simulations

The code has been tested for several parameters sets.

- Iterations increase slightly when the number of refinements is increased;
- continuous solutions, but non-matching values at the boundary.

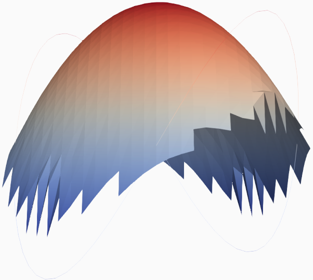

Figure 3: Bulk and surface solutions.

How to improve the code?

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- generalize to non-constant parameters;
- check the expected convergence rate of the method;

Possible extensions

Avenues for future work:

- Add a constraint to find the solution we want;
- parallelization;
- generalize to non-constant parameters;
- check the expected convergence rate of the method;
- stabilize the surface equation.

Appendix

Laplace-Beltrami operator and curvature

For a twice differentiable function $f : \Gamma \to \mathbb{R}$, the Laplace-Beltrami operator is defined as

$$\Delta_\Gamma f = \nabla_\Gamma \cdot \nabla_\Gamma f.$$

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We can write

$$\Delta_\Gamma f = \Delta \tilde{f} \underbrace{-\nabla \cdot \left(\left(\boldsymbol{n} \cdot \nabla \tilde{f} \right) \boldsymbol{n} \right)}_{A} - \left(\mathrm{H} (\tilde{f})\ \boldsymbol{n} \right) \cdot \boldsymbol{n} + \underbrace{\nabla \left(\left(\boldsymbol{n} \otimes \boldsymbol{n} \right) \nabla f \right) \boldsymbol{n} \cdot \boldsymbol{n}}_{B}.$$

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Here,

$$\begin{aligned} A &= -\nabla \left(\boldsymbol{n} \cdot \nabla \tilde{f} \right) \cdot \boldsymbol{n} - \left(\boldsymbol{n} \cdot \nabla \tilde{f} \right) \left(\nabla \cdot \boldsymbol{n} \right) \\ &= - \left(\mathrm{H}(\tilde{f})\ \boldsymbol{n} \right) \cdot \boldsymbol{n} - \left(\nabla \boldsymbol{n} \right) \boldsymbol{n} \cdot \nabla \tilde{f} - \left(\boldsymbol{n} \cdot \nabla \tilde{f} \right) \left(\nabla \cdot \boldsymbol{n} \right). \end{aligned}$$

Laplace-Beltrami operator and curvature

Similarly,

$$B = \left(\mathrm{H}(\tilde{f})\, \boldsymbol{n}\right) \cdot \boldsymbol{n} + (\nabla \boldsymbol{n})\, \boldsymbol{n} \cdot \nabla \tilde{f} + \left(\boldsymbol{n} \cdot \nabla \tilde{f}\right) ((\nabla \boldsymbol{n})\, \boldsymbol{n} \cdot \boldsymbol{n})\,.$$

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Remark 1: the Laplace-Beltrami operator strongly depends on the geometry.

Laplace-Beltrami operator and curvature

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Remark 1: the Laplace-Beltrami operator strongly depends on the geometry.

Remark 2: if $\boldsymbol{n}$ has constant length, then the term $(\nabla \boldsymbol{n})\,\boldsymbol{n} \cdot \boldsymbol{n}$ vanishes.

Useful inequalities

Here, a couple of useful relations are reported.

- For continuity of the model problem bilinear form:

$$|a_1||a_2| + |b_1||b_2| \leq \sqrt{2}\left(|a_1|^2 + |b_1|^2\right)^{1/2}\left(|a_2|^2 + |b_2|^2\right)^{1/2}$$

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- For coercivity of the model problem bilinear form:
  Poincaré-Wirtinger inequality: let $f \in H^1(D)$. Then, there exists $c_D > 0$ such that

$$\|f - f_D\|_{L^2(D)} \leq c_D \|\nabla f\|_{L^2(D)},$$

  where

$$f_D = \frac{1}{|D|}\int_D f(x)\,\mathrm{d}x.$$

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