Coupling strategies, non-matching methods, and dimensionality reduction across heterogeneous dimensions

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deal.II and me (+ collaborators* and friends*!)

some deal.II contributions

- Co-dimensions
- Manifold
- MappingFEField
- BEM support (*)
- MeshLoop (*)
- ParameterAcceptor
- GridTools::Cache
- Non-matching stuff
- insert global particles (*)
- ScratchData
- FECouplingValues

Interfaces to external libraries

- FunctionParser
- OpenCASCADE
- Assimp
- KDTree(Nanoflann)
- rtree(boost)
- SUNDIALS
- GMSH Api
- CGAL
- PETSc TS (*)
- PETSc SNES (*)

Infrastructure

- docker Images
- MAC Packages

Tutorial programs (*)

- step-34
- step-53
- step-54
- step-60
- step-70
- step-80 (soon!)

Coupling?

Simplest form of coupling: boundary conditions

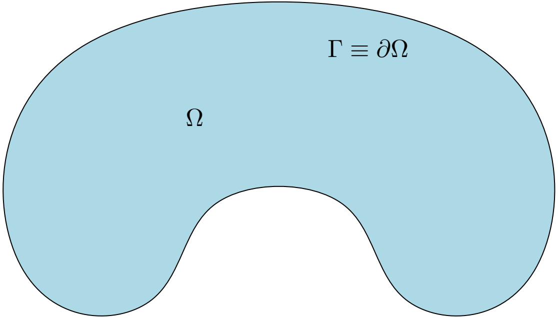
$$\begin{aligned} -\Delta u &= f \qquad \text{in } \Omega \\ u &= g \qquad \text{on } \Gamma \end{aligned}$$

Lagrange multipliers (Babuska 1973)

$$(\nabla u, \nabla v) + < \lambda, v > = (f, v) \qquad \forall v \in V = H^1(\Omega)$$

$$< u, q > = < g, q > \qquad \forall q \in Q = H^{-\frac{1}{2}}(\Gamma)$$

Ivo Babuska. The finite element method with lagrangian multipliers.
Numerische Mathematik, 20(3):179–192, June 1973




```
Triangulation<dim> omega;
Triangulation<dim-1, dim> gamma;
// ...
GridGenerator::extract_boundary_mesh
                    (omega, gamma, {0});
```

`Triangulation` is easy (see `step-38`). How about `DoFHanlder`?

- ✓ "Easy" to extract co-dimension one triangulations
- ✗ non-trivial (prior to v9.6.0) to match dof iterators

```
Triangulation<dim> omega;
Triangulation<dim-1, dim> gamma;
// ... generate omega ...
const auto surface_to_bulk_map =
  GridGenerator::extract_boundary_mesh(omega, gamma, {0});

omega_dof_handler.distribute_dofs(fe);
gamma_dof_handler.distribute_dofs(surface_fe);

// Extract the mapping between surface and bulk degrees of freedom:
// std::map< typename DoFHandler< dim - 1, spacedim >::active_cell_iterator,
//           std::pair< typename DoFHandler< dim, spacedim >::active_cell_iterator,
     unsigned int > >
const auto surface_to_bulk_dof_iterator_map =
  DoFTools::map_boundary_to_bulk_dof_iterators(surface_to_bulk_map,
                                               omega_dof_handler,
                                               gamma_dof_handler);
```

Now we have cell iterators. How about `FEValues`?

```
FEFaceValues<dim>          fv1(bulk_fe, quad, update_flags);
FEValues<dim-1, spacedim> fv2(surface_fe, quad, update_flags);
// ...
for(const auto &surface_cell : gamma_dof_handler.active_cell_iterators()) {
  auto [cell1, face] = surface_to_bulk_dof_iterator_map[surface_cell];

  fv1.reinit(cell1, face);
  fv2.reinit(cell2);

  FECouplingValues<dim, dim-1, spacedim> fcv(fv1, fv2, DoFCouplingType::contiguous,
                                            QuadratureCouplingType::matching);

  const auto bulk    = fcv.get_first_extractor(scalar);
  const auto surface = fcv.get_second_extractor(scalar);

      // ...
      const auto &bulk_vi    = fcv[bulk].value(i, q);
      const auto &surface_vi = fcv[surface].value(i, q);
      // ...
}
```

Cahn-Hilliard example

Given a bounded domain $\mathscr{P} \in \mathbb{R}^{2,3}$, the standard Cahn-Hilliard equations [28] reads:

$$\begin{cases} \dot{\varphi}_{\mathscr{P}} = m_{\mathscr{P}} \triangle \mu_{\mathscr{P}}, & \text{in } \mathscr{P}, \\ \mu_{\mathscr{P}} = -\varepsilon \triangle \varphi_{\mathscr{P}} + \frac{1}{\varepsilon} f'(\varphi_{\mathscr{P}}), & \text{in } \mathscr{P}, \end{cases}$$

where $\varphi_{\mathscr{P}}$ defines the phase field, $\mu_{\mathscr{P}}$ the chemical potential, $m_{\mathscr{P}} > 0$ is the mobility, and ε is a parameter controlling the thickness of the interface between phases. f is the potential, usually the double-well: $\frac{1}{4}(p^2 - 1)^2$.

John W Cahn and John E Hilliard. Free energy of a nonuniform system. i. interfacial free energy. *The Journal of chemical physics*, 28(2):258–267, 1958

Bulk-Surface couplings

Better description of short-range interactions between the bulk and its boundary:

$$\begin{cases} \dot{\varphi}_{\mathscr{P}} = s_{\mathscr{P}} + m_{\mathscr{P}} \triangle \mu_{\mathscr{P}}, & \text{in } \mathscr{P} \\ \mu_{\mathscr{P}} = -\varepsilon \triangle \varphi_{\mathscr{P}} + \frac{1}{\varepsilon} f'(\varphi_{\mathscr{P}}) - \gamma, & \text{in } \mathscr{P}, \\ \dot{\varphi}_{\partial\mathscr{P}} = s_{\partial\mathscr{P}} + m_{\partial\mathscr{P}} \triangle_{\mathscr{S}} \mu_{\partial\mathscr{P}} - \beta m_{\mathscr{P}} \partial_n \mu_{\mathscr{P}}, & \text{on } \partial\mathscr{P}, \\ \mu_{\partial\mathscr{P}} = -\imath \delta \triangle_{\mathscr{S}} \mu_{\partial\mathscr{P}} + \frac{1}{\delta} g'(\varphi_{\partial\mathscr{P}}) + \varepsilon \partial_n \varphi_{\mathscr{P}} - \zeta & \text{on } \partial\mathscr{P}, \end{cases}$$

where $s_{\mathscr{P}}, s_{\partial\mathscr{P}}$ are the external rates of species production, γ an external bulk microforce, and ζ an external surface microforce.

Luis Espath. A continuum framework for phase field with bulk-surface dynamics.
Partial Differential Equations and Applications, 4(1):1, 2023

Boundary conditions

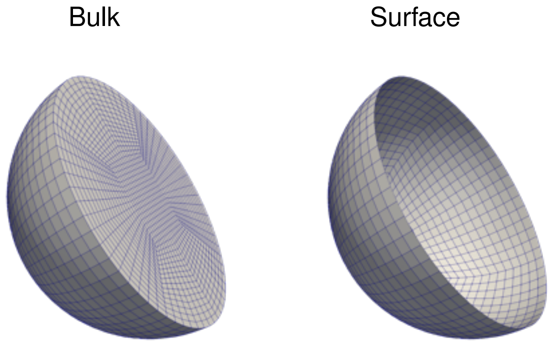
$\partial\mathscr{P} := \partial\mathscr{P}^{\mathrm{dyn}} \cup \partial\mathscr{P}^{\mathrm{sta}}$ and $\partial\mathscr{P}^{\mathrm{dyn}} \cap \partial\mathscr{P}^{\mathrm{sta}} = \varnothing$:

$$\forall \boldsymbol{x} \in \partial\mathscr{P}^{\mathrm{dyn}} \begin{cases} \varphi_{\mathscr{P}} = \varphi_{\partial\mathscr{P}}, \qquad \text{or} \qquad \varepsilon\,\partial_n \varphi_{\mathscr{P}} = \frac{1}{L_\varphi}(\dot{\varphi}_{\partial\mathscr{P}} - \dot{\varphi}_{\mathscr{P}}), \\ \mu_{\mathscr{P}} = \beta\mu_{\partial\mathscr{P}}, \qquad \text{or} \qquad -m_{\mathscr{P}}\,\partial_n \mu_{\mathscr{P}} = -\frac{1}{L_\mu}(\beta\mu_{\partial\mathscr{P}} - \mu_{\mathscr{P}}), \end{cases}$$

and

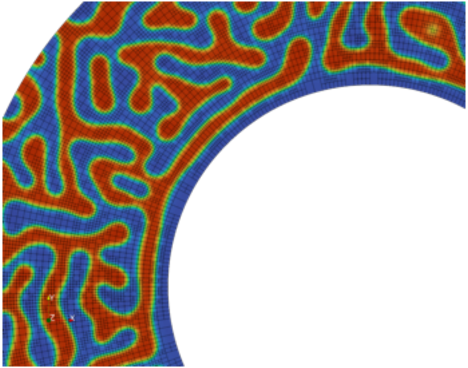
$$\forall \boldsymbol{x} \in \partial\mathscr{P}^{\mathrm{sta}} \begin{cases} \varphi_{\mathscr{P}} = \varphi^{\mathrm{env}}_{\partial\mathscr{P}}, \qquad \text{or} \qquad \varepsilon\,\partial_n \varphi_{\mathscr{P}} = \xi^{\mathrm{env}}_{\mathscr{S}}, \\ \mu_{\mathscr{P}} = \mu^{\mathrm{env}}_{\partial\mathscr{P}}, \qquad \text{or} \qquad -m_{\mathscr{P}}\,\partial_n \mu_{\mathscr{P}} = -\iota^{\mathrm{env}}_{\partial\mathscr{P}}, \end{cases}$$

Numerical challenges



- Separate meshes for bulk and surface
- Potentially very large nonlinear systems of algebraic differential equations

Numerical challenges



- Adaptive mesh refinement.
- Nonlinear time steppers for Differential-Algebraic-Equations.
- Adaptive time stepping.

deal.II - PETSc DAE wrapper

Given the implicit DAE:

$$F(t, u, \dot{u}) = 0$$

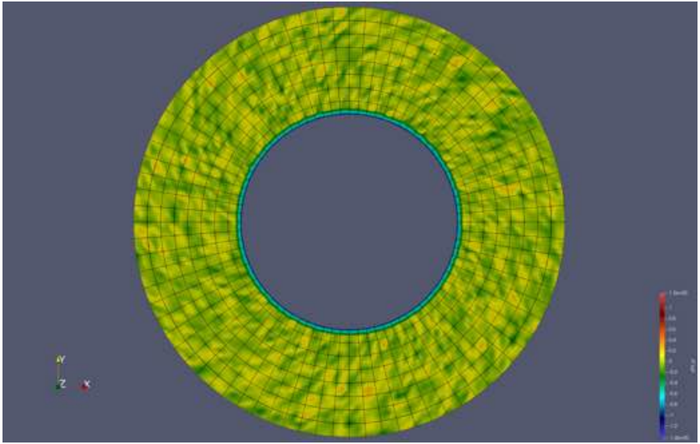
PETSc expects users to provide

- The residual evaluation for a given $(t, u, \dot{u})$ input (essential boundary conditions strongly imposed).
- The Jacobian $\sigma \frac{\partial F}{\partial \dot{u}} + \frac{\partial F}{\partial u}$, which in our case reads (modulo BC):

$$\sigma \begin{pmatrix} \boldsymbol{M} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & M & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & m_{\mathscr{P}} \boldsymbol{K} & 0 & 0 \\ -\varepsilon \boldsymbol{K} - \frac{1}{\varepsilon} \boldsymbol{J}_1 & \boldsymbol{M} & 0 & 0 \\ 0 & m_{\mathscr{P}} \boldsymbol{C} & 0 & \beta m_{\partial \mathscr{P}} K \\ -\varepsilon \boldsymbol{C} & 0 & -\iota \delta K - \frac{1}{\delta} J_2 & M \end{pmatrix}$$

Preliminary 2D results

Using BDF2 and adaptive time stepping based on digital signal processing [24].



General coupling problem

Abstract formulation

$$\int_A \int_B v(x) K(x,y) u(y) \mathrm{d}x \mathrm{d}y$$

- A and B are two (possibly) independent domains, with (possibly) different co-dimensions
- $K(x,y)$ is a (possibly singular) kernel
- When K is the Dirac delta distribution, the integral above becomes formally:

$$\int_{\bar{A} \cap \bar{B}} v(x) u(x) \mathrm{d}(\bar{A} \cap \bar{B})$$

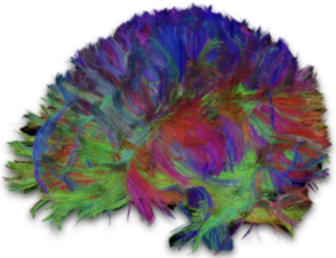
`FECouplingValues` is designed to help in treating the above abstract formulation

My driving motivation: mechanical properties of living tissues

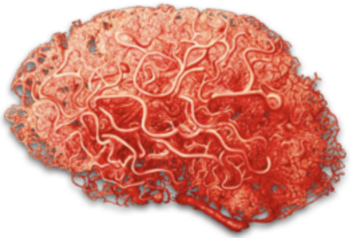
Example: the brain:

- Complex and feature-rich geometry
- Non-linear poro-visco-elastic material, anisotropic, inhomogeneous
- Immersed in (moving) Cerebro-Spinal Fluid (CSF)
- Perfused with pulsating blood

Grey matter +



Axons +



Vasculature

The case for multiscale-multiphysics-multidimensional coupling

Slender structures

- ✓ Axons and vessels are slender structures
  - ✓ We need consistent ways to reduce the *geometric* dimensionality
  - ✗ When reducing the dimensionality, traces my stop being meaningful (coupling is complicated)

Multi-scale

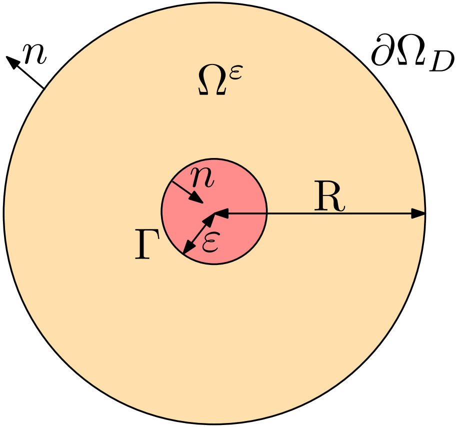
- ✓ The relative dimension of a single axon (vessel) w.r.t. the domain is negligible (microscale)
- ✗ The number of inclusions/axons/vessels is large
  (their meso- and macro- scopic effect is **not** negligible)

Multi-physics

- ✓ Axons and Vessels should be modeled differently from the Grey matter
  - ✓ Axons: electrical activation, electro-mechanical coupling
  - ✓ Blood vessels: fluid flow, fluid-structure interaction

What can go wrong?

A very simple example: one blood vessel, diffusion of oxygen concentration (u)



- B_ε: Blood vessel (cylinder of radius ε)
- $\Omega^\varepsilon := B_R \setminus B_\varepsilon$: Brain tissue (cylinder of radius R, minus the vessel)
- $\Gamma := \partial B_\varepsilon$: Surface of the vessel

Linear diffusion – 2D slice

$$\begin{aligned} -\Delta u &= 0 && \text{in } \Omega^\varepsilon && := && B_R \setminus B_\varepsilon \\ u &= 0 && \text{on } \partial\Omega_D && := && \partial B_R \\ u &= g && \text{on } \Gamma && := && \partial B_\varepsilon, \end{aligned}$$

Exact solution (g constant):

$$u(r) = g\frac{\ln(r) - \ln(R)}{\ln(\varepsilon) - \ln(R)}$$

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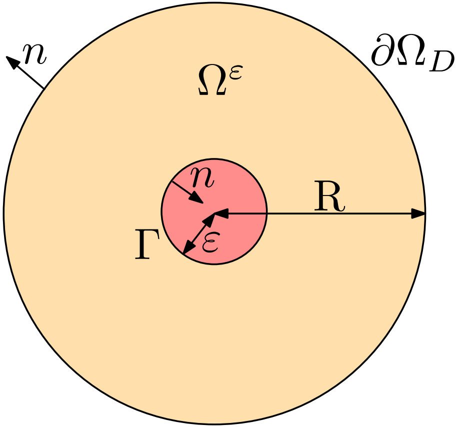

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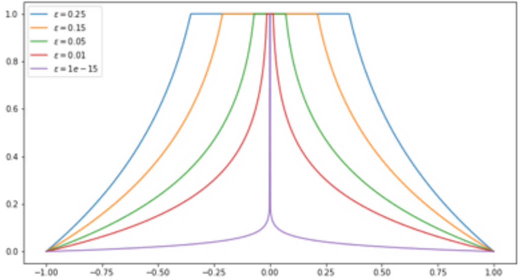


Taking the limit for $\varepsilon \to 0$ is NOT physical

- ✗ Limit of u for $\varepsilon \to 0$ (with g **constant**):

$$\lim_{\varepsilon \to 0} u = \begin{cases} u = 0 & x \in \Omega \setminus 0 \\ u = g & x = 0 \end{cases}$$

- ✓ A more meaningful approach: keep ε fixed (i.e., **impose, somehow, the condition** $u \sim g$ **on** ∂B_ε), but "fill" the hole B_ε with something sensible/useful/meaningful
  - ✗ Singular option: fill the hole with a fundamental solution, i.e., locally the solution to

$$-\Delta u = c\delta$$

    where c is chosen so that $u \sim g$ on ∂B_ε (optionally **split** solution in **regular** and **singular** parts)
  - ✓ Regularized option: fill the hole with a regularized fundamental solution, i.e., locally the solution to

$$-\Delta u = c\delta^\rho$$

    where c is chosen so that $u \sim g$ on ∂B_ε, and δ^ρ is a smooth approximation of δ
  - ✓ Lagrange multiplier option (**more later**)

Geometric dimensionality reduction

A slender structure $\Omega \subseteq R^d$

✓ Ω is well represented by a subset γ of Ω whose intrinsic dimension is smaller than d

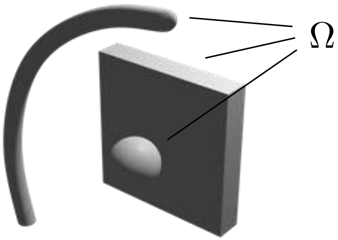
- e.g.: a representative surface γ
- e.g.: a representative curve γ
- e.g.: a representative point γ

Assume we can apply Fubini's theorem

For any absolutely integral f, we must be able to write

$$\int_\Omega f \mathrm{d}\Omega = \int_\gamma \int_D f \mathrm{d}D \mathrm{d}\gamma$$

$D(s)$ is the cross-section of Ω at a point $s \in \gamma$.



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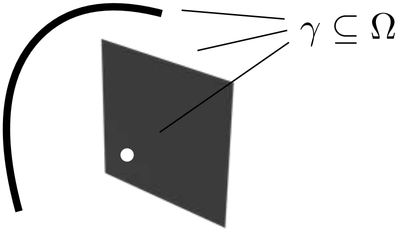


 Geometric dimensionality reduction

Infinite dimensional dimensionality reduction

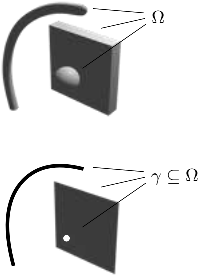
Main idea

- ✓ Given a domain Ω and a representative subset γ of Ω
- ✓ Define basis functions φ_i with "good" properties along the sections D ("orthogonal" to γ) of $\Omega = \gamma \times D$ (i.e., $\nabla_\gamma \varphi_i \equiv 0$ in Ω, and polynomial or trigonometric along D)
- ✓ Keep infinite dimensional representation on γ, and finite dimensional on D, i.e.,
  - ✓ Define a geometric projection operator Π from Ω to γ
  - ✓ Define a φ_i-weighted extension operator $\mathscr{E}^i$ from γ to Ω
  - ✓ Define a φ_i-weighted average operator $\mathscr{A}^i$ from Ω to γ

Main result

- ✓ The operators $\mathscr{E}^i$ and $\mathscr{A}^i$ are bounded and admit a bounded left and right inverse
- ✓ $\mathscr{E}^i$ and $\mathscr{A}^i$ allow to define a consistent way to transfer information between V and γ
- ✓ $\mathscr{E}^i$ and $\mathscr{A}^i$ define a consistent way to reduce the dimensionality of the problem

Projection, weighted average, and weighted extension



Geometric projection

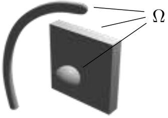
$$
\begin{aligned}
\Pi : \quad & \Omega \mapsto \quad \gamma \\
\Pi^{-1} : \quad & \gamma \mapsto \quad \mathscr{P}(\Omega)
\end{aligned}
$$

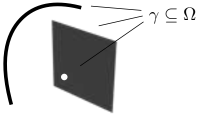
For simplicity assume that $D(s) := \int_{\Pi^{-1}(s)} \mathrm{d}\mathscr{H}(\Pi^{-1})$ is > 0 for each $s \in \gamma$ and that it has always the same intrinsic dimension:

$$
\int_{\Omega} f \mathrm{d}\Omega = \int_{\gamma} \int_{D} f \mathrm{d}D \mathrm{d}\gamma
$$

Geometric dimensionality reduction

Projection, weighted average, and weighted extension





Weighted Average and Weighted Extension

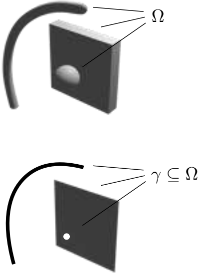
$$(\mathscr{A}^0 f)(s) := \frac{1}{|D(s)|} \int_{D(s)} f \mathrm{d}D(s) =: \left(\fint_D f \mathrm{d}D \right)(s), \quad s \in \gamma$$

$$(\mathscr{E}^0 w)(x) := (w \circ \Pi)(x)$$

$$\mathscr{A}^0 \mathscr{E}^0 w = \delta_{ij} w, \qquad \forall w \in C^0(\overline{\gamma})$$

Geometric dimensionality reduction

Projection, weighted average, and weighted extension



Weighted Average and Weighted Extension

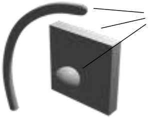
$$(\mathscr{A}^i f)(s) := \frac{1}{|D(s)|}\int_{D(s)} f \mathrm{d}D(s) =: \left(\fint_D \varphi_i f \mathrm{d}D\right)(s), \quad s \in \gamma$$

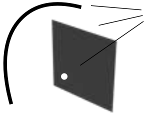
$$(\mathscr{E}^i w)(x) := \varphi_i(x)(w \circ \Pi)(x)$$

$\varphi_0 = 1, \qquad \varphi_i(x) \qquad$ s.t. $\qquad \nabla_\gamma \varphi_i \equiv 0, \qquad$ and

$$\mathscr{A}^i \mathscr{E}^j w = \delta_{ij} w, \qquad \forall w \in C^0(\overline{\gamma})$$

Projection, weighted average, and weighted extension





Extension operator (LH Zunino 2023)

$$R^T : \qquad H^s(\gamma)^N \mapsto \quad H^s(\Omega) \qquad s \in [-1, 1]$$

$$w \to R^T w := \sum_{i=0}^{N-1} \mathscr{E}^i w_i$$

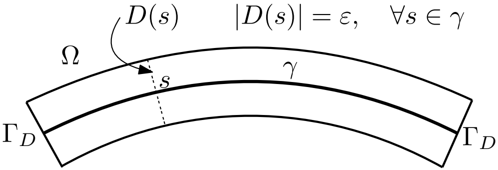
is bounded and admits a bounded right inverse, under reasonable geometrical assumptions on Ω and γ.

Equivalently:

- ✓ $R^T(H^s(\gamma)^N) =: V_\gamma$ is a closed subspace of $H^s(\Omega)$
- ✓ $\exists \beta > 0$ s.t. $\|R^T w\|_{s,\Omega} \geq \beta \|w\|_{s,\gamma}$
- ✓ R and R^T satisfy an *infsup* condition

 Geometric dimensionality reduction

Example of consistent dimensionality reduction



Weak Poisson problem

Find $u \in V := H^1_{0,\Gamma_D}(\Omega)$ such that

$$\int_\Omega \nabla u \nabla v \, d\Omega = \int_\Omega f v \, d\Omega \qquad \forall v \in V$$

$$Au = f \qquad \text{in } V'$$

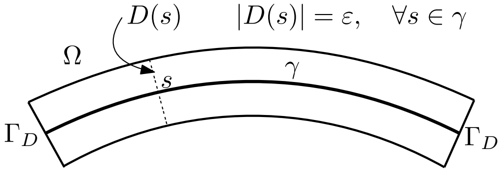
Weak reduced Poisson problem

Find $u_\gamma \in V_\gamma := R^T(H^1_{s,0}(\gamma))$ such that

$$\int_\Omega \nabla u_\gamma \nabla v_\gamma \, d\Omega = \int_\Omega f v_\gamma \, d\Omega \qquad \forall v_\gamma \in V_\gamma$$

$$Au_\gamma = f \qquad \text{in } V'_\gamma$$

Example of consistent dimensionality reduction



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$$Au_\gamma = f \qquad \text{in } V'_\gamma$$

Properties of the reduced Poisson problem - I

From standard Ritz-Galerkin theory

- ✓ V_γ is a closed subspace of V implies

$$\|u-u_\gamma\|_{H^1(\Omega)} \leq C \inf_{v_\gamma \in V_\gamma} \|u-v_\gamma\|_{H^1(\Omega)}$$

- ✓ R^T admits a bounded right inverse implies

$$\forall v_\gamma \in V_\gamma \quad \exists! w \in H^1_0(\gamma) \quad \text{s.t.} \quad R^T w = v_\gamma$$

- ✓

$$Au_\gamma = f \text{ in } V'_\gamma \quad \Longleftrightarrow \quad RAR^T w = Rf \qquad \text{in } H^{-1}(\gamma)$$

- ✓ φ_i is complete orthonormal basis for D implies

$$\lim_{N\to\infty} \inf_{v_\gamma \in V_\gamma} \|u-v_\gamma\|_{H^1(\Omega)} = 0$$

Properties of the reduced Poisson problem - II

- ✓ $N = 1$ implies using only $\varphi_0 = 1$: V_γ is the space of functions that are constant on a *tubular extension of* γ
  - ✓ The Poisson problem reduces to a Laplace-Beltrami problem on γ
  - ✓ Replacing u with u_γ in the original problem entails an error that is of order ε in $H^1(\Omega)$
- ✓ If we need a finer representation, we can increase N
- ✓ This formulation is still infinite dimensional on γ
- ✓ Since we do not change the problem on Ω, but just the functional space, we never face the issue of traces on γ (which are always defined through R^T)
- ✓ The choice of φ_i is crucial, and it is the only thing that we have freedom to choose (i.e., Fourier basis, Polynomial basis, etc.). Different choices will lead to different reduced problems

Dimensionality Reduction error in H^s

$$E_{s,\gamma} := \sup_{u \in H^s(\Omega)} \inf_{v_\gamma \in V_\gamma} \|u - v_\gamma\|_{s,\Omega} = e(\varepsilon := |D|, N, \Omega, \gamma, s)$$

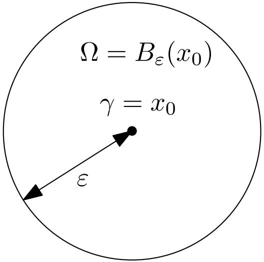
More “extreme” restriction operator

Spherical harmonic restriction – 2D – 0D

$$< Ru, w >:= w^i \int_\Omega \varphi_i u \mathrm{d}\Omega \qquad \forall u \in V \equiv H^1(\Omega), \qquad \forall w \in \Re^N$$

where φ_i are spherical harmonics on $B_\varepsilon(x_0)$.

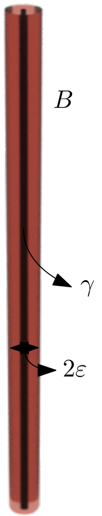
- ✓ When $N = 1$, $R^T w$ is a constant function on Ω with value w
- ✓ We replace u with a projection onto the spherical harmonics of u, i.e., *the best spherical harmonic approximation of u*



Fourier extension on cylinders

To fix the ideas

- Single cylinder aligned with the x_3-axis
- Radius ε
- P_γ: project any point x in B to its closest point $\hat{x}$ on γ (for a straight cylinder: $P_\gamma(x_1, x_2, x_3) = x_3 \equiv \hat{x}$)
- $\varphi_n(x) = \varphi_n(x_1, x_2)$: harmonic functions on the *fixed two dimensional cross section* $D_{\hat{x}}$ of B, for $n = 1, \ldots, N$



Harmonic extension operator on reference cylinder

$$(R^T w_\gamma)(x) := \sum_{i=1}^{N} w_\gamma^i(P_\gamma(x))\varphi_i(x)$$

Fourier extension on cylinders

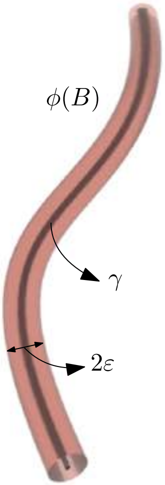
- ϕ: diffeomorphism of B

Harmonic extension operator on $\phi(B)$

$$(R^T w_\gamma)(x) := \sum_{i=1}^{N} w_\gamma^i(P_\gamma(x))\varphi_i(\phi^{-1}(x))$$

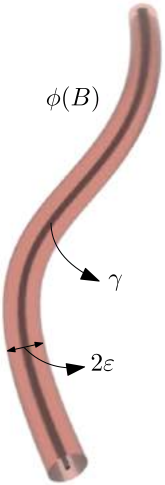
Reduction error ($n =$ number of Fourier modes, $N = 2n+1$):

$$E_{s,\gamma} := \sup_{u \in H^s(\Omega)} \inf_{v_\gamma \in V_\gamma} \|u - v_\gamma\|_{H^1(\Omega)} \leq C\varepsilon^{n+1} |u|_{n+2,\Omega}$$

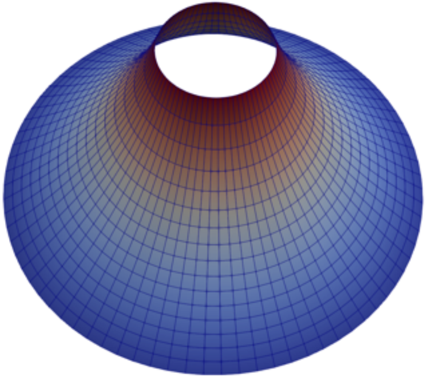


Fourier extension on cylinders

How about coupling with a 3D problem?



Back to Babuska



Strong imposition of boundary conditions

Find u, u_h, in $H^1(\Omega^\varepsilon)$ satisfying BC, such that:

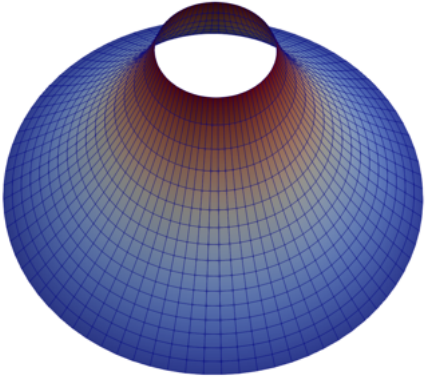
$$
\begin{aligned}
(\nabla u, \nabla v) = 0 \quad & \forall v \in V_0 \equiv H^1_{0,\partial\Omega_D}(\Omega^\varepsilon) \\
(\nabla u_h, \nabla v_h) = 0 \quad & \forall v \in V_{h,0} \subset V_0
\end{aligned}
$$

Imposition of BC using a Lagrange multiplier

$$
\begin{aligned}
\mathscr{A}u \quad +\mathscr{C}^T\lambda \quad &= f_1 \qquad \text{in } V'(\Omega^\varepsilon) \\
\mathscr{C}u \quad &= g \qquad \text{in } Q'(\Gamma)
\end{aligned}
$$

The Lagrange multiplier λ can be seen as a "forcing term" to add in order to impose that the solution u is equal to g on Γ. $\lambda = -\partial u/\partial n$

Back to Babuska



Strong imposition of boundary conditions

Find u, u_h, in $H^1(\Omega^\varepsilon)$ satisfying BC, such that:

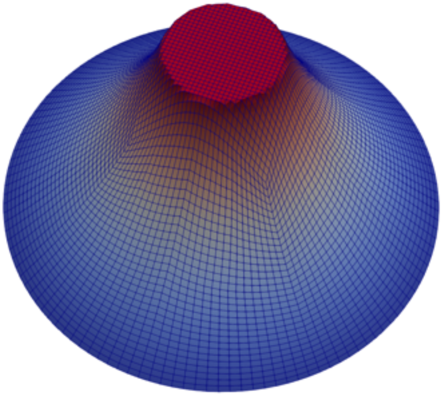
$$\mathscr{A} u = f \quad \text{in } V_0'$$

Imposition of BC using a Lagrange multiplier

$$\begin{aligned} \mathscr{A} u \quad + \mathscr{C}^T \lambda \quad &= f_1 \qquad && \text{in } V'(\Omega^\varepsilon) \\ \mathscr{C} u \quad &= g && \text{in } Q'(\Gamma) \end{aligned}$$

The Lagrange multiplier λ can be seen as a “forcing term” to add in order to impose that the solution u is equal to g on Γ. $\lambda = -\partial u / \partial n$

Fictitious domain solution (2D-3D coupling)



Imposition of internal BC using a Lagrange multiplier

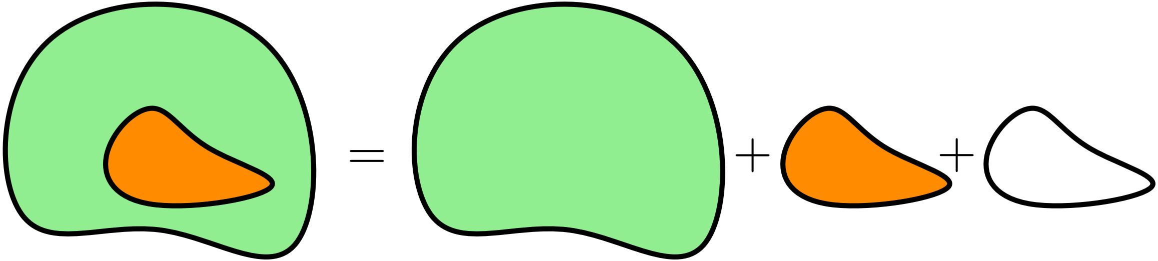
$$
\begin{aligned}
\mathscr{A}u \quad + \mathscr{C}^T\lambda \quad &= f_1 \qquad \text{in } V'(\Omega)\\
\mathscr{C}u \quad &= g \qquad \text{in } Q'(\Gamma)
\end{aligned}
$$

- ✓ Γ does not need to be aligned with the grid of Ω
- ✗ The regularity of the global solution is smaller w.r.t. to the previous case
- ✗ The Lagrange multiplier is in the dual of the space of traces of V on Γ, i.e., $H^{-1/2}(\Gamma)$
- ✓ The loss of regularity is a local phenomenon (LH N. Rotundo 2019)

The Lagrange multiplier λ is again a "forcing term" to add in order to impose that the solution u is equal to g on Γ. $\lambda = -\partial u^+/\partial n + \partial u^-/\partial n$

Graphical summary of non-matching methods

Lagrange multipliers (AKA fictitious domain method)



- ✓ Extend background equations to whole domain
- ✓ Solve foreground problem on separate domain
- ✓ Impose transmission and boundary conditions through a Lagrange multiplier *on the interface*
- ✗ We need a numerically efficient way to transfer information between the interface (possibly non-matching) and the background domain

Historical overview

- Imposing boundary conditions with Lagrange multipliers
  - Ivo Babuska. The finite element method with lagrangian multipliers. *Numerische Mathematik*, 20(3):179–192, June 1973
  - James H. Bramble. The lagrange multiplier method for dirichlet's problem. *Mathematics of Computation*, 37(155):1, July 1981
- Fictitious domain methods
  - Roland Glowinski, Tsorng-Whay Pan, and Jacques Périaux. A fictitious domain method for dirichlet problem and applications. *Computer Methods in Applied Mechanics and Engineering*, 111:283–303, 1994
- . . . many more . . .
- Local regularity estimates via weighted spaces
  - LH and Nella Rotundo. Error estimates in weighted sobolev norms for finite element immersed interface methods. *Computers and Mathematics with Applications*, 2019

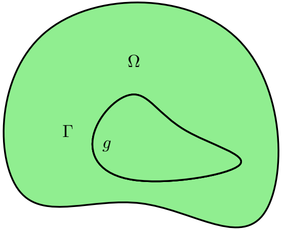
Fictitious Domain Method (FDM)

Original problem (to fix the ideas)

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega \setminus B \\ u &= g && \text{on } \Gamma \end{aligned}$$

Extended non-matching problem with Lagrange multiplier

$$\begin{aligned} (\nabla u, \nabla v)_\Omega + < \lambda, v >_\Gamma &= (f, v) && \forall v \in V(\Omega) \equiv H^1_0(\Omega) \\ < u, q >_\Gamma &= < g, q > && \forall q \in Q(\Gamma) \equiv H^{-1/2}(\Gamma) \end{aligned}$$



Operatorial form (A is weak Laplacian, B is trace operator)

$$\begin{aligned} Au \quad + B^T\lambda &= f && \text{in } V'(\Omega) \\ Bu \quad &= g && \text{in } Q'(\Gamma) \end{aligned}$$

Reduced Lagrange multiplier formulation

Infinite dimensional restriction

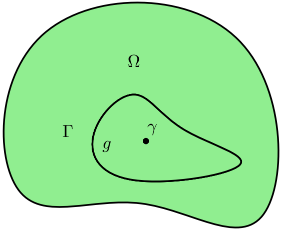
Fully resolved formulation

$$
\begin{aligned}
Au \quad +B^T\lambda &= f \qquad \text{in } V'(\Omega)\\
Bu \qquad\qquad &= g \qquad \text{in } Q'(\Gamma)
\end{aligned}
$$

Reduced formulation

$$
\begin{aligned}
Au_\gamma \quad +B^TR^T\Lambda &= f \qquad \text{in } V'(\Omega)\\
RBu \qquad\qquad &= Rg \qquad \text{in } Q'_\gamma(\gamma)
\end{aligned}
$$

Same as restricting λ to the image of R^T, i.e., searching for a $\lambda_\gamma \in R^TQ_\gamma \subset Q$ instead of $\lambda \in Q$



Classical hypotheses on A and B

Ell-Ker

$$\exists \alpha \text{ s.t. } \inf_{u \in \mathrm{Ker}(B)} \sup_{v \in \mathrm{Ker}(B)} \frac{< Au, v >}{\|u\|_V \|v\|_V} \geq \alpha > 0$$

Inf-Sup

$$\exists \beta \text{ s.t. } \inf_{v \in \mathrm{Ker}(B)^\perp} \sup_{\lambda \in Q \setminus \ker(B^T)} \frac{< Bv, \lambda >}{\|v\|_V \|\lambda\|_Q} \geq \beta > 0$$

- ✓ Ell-Ker follows from coercivity of A
- ✓ Inf-Sup follows from trace Theorem

Daniele Boffi, Franco Brezzi, and Michel Fortin. *Mixed Finite Element Methods and Applications*, volume 44 of *Springer Series in Computational Mathematics*.
Springer Berlin Heidelberg, Berlin, Heidelberg, 2013

Dimensionality reduction error (LH Zunino 2023)

Error due to dimensionality reduction (continuous problem)

$$\|u - u_\gamma\|_V \leq \frac{\|B^T\|}{\alpha} \inf_{w \in Q_\gamma} \|\lambda - R^T w\|_Q \leq C_1 E_R$$

$$\|\lambda - R^T \Lambda\| \leq \left(1 + \frac{2\|A\|\|B^T\|\|R^T\|}{\alpha \beta_R \beta}\right) \inf_{w \in Q_\gamma} \|\lambda - R^T w\|_Q \leq C_2 E_R$$

$$E_R := \inf_{w \in Q_\gamma} \|\lambda - R^T w\|_Q$$

Follows from standard saddle point theory:

Daniele Boffi, Franco Brezzi, and Michel Fortin. *Mixed Finite Element Methods and Applications*, volume 44 of *Springer Series in Computational Mathematics*.
Springer Berlin Heidelberg, Berlin, Heidelberg, 2013

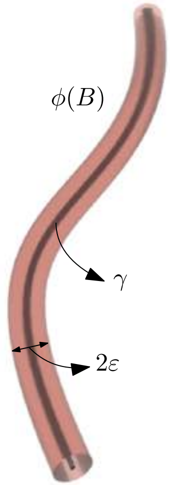
Reduced Lagrange multiplier error estimate (LH Zunino 2023)

Theorem (LH Paolo Zunino, 2023)

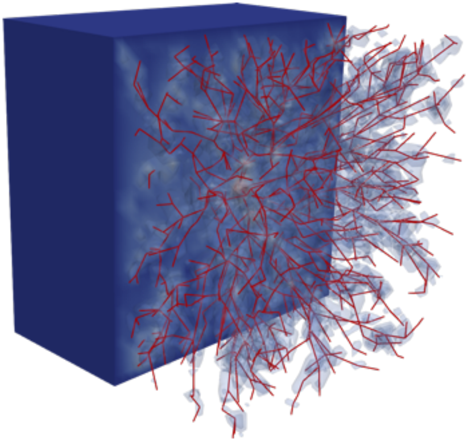
$$
\|u - u_{R,h}\|_{1,\Omega} \leq C_1 \left(\frac{\varepsilon}{\delta}\right)^{n+1} + C_2 \left(1 + \frac{h}{\varepsilon}\right)^{n} \inf_{v \in V_h} \|u - v_h\|_{1,\Omega} + C_3 \inf_{\lambda_h \in Q_h} \|\lambda - \lambda_h\|_{-1/2,\Gamma}
$$

$$
\|\lambda - \Lambda_h\|_{-1/2,\Gamma} \leq C_4 \left(\frac{\varepsilon}{\delta}\right)^{n+1} + C_5 \left(1 + \frac{h}{\varepsilon}\right)^{2n} \inf_{v \in V_h} \|u - v_h\|_{1,\Omega} + C_6 \left(\frac{\varepsilon}{\delta}\right)^{n} \inf_{\lambda_h \in Q_h} \|\lambda - \lambda_h\|_{-1/2,\Gamma}
$$

- δ: min distance between vessels
- $n \leq k$: number of Fourier modes
- k: polynomial degree of the approximation space



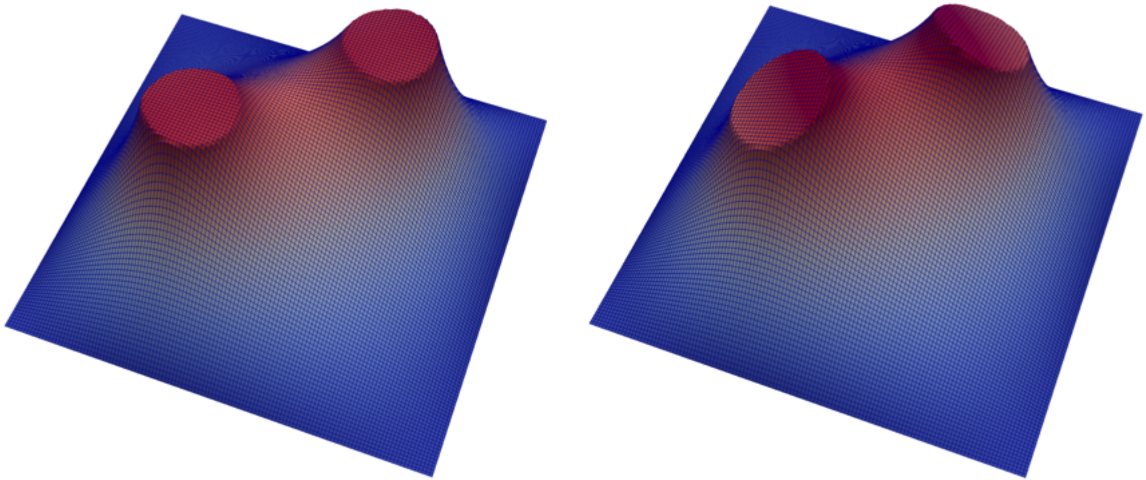
Why fictitious domain methods / non-matching methods?



- Real life blood networks are very complicated
  - ✗ meshing the space between vessels may be computationally impossible
  - ✗ even if we could, the quality of the mesh could be very bad
  - ✗ the resulting grid may be too coarse anyway
- Even if we don't capture the full details of the blood network with a uniformly refined grid:
  - ✓ the presence of the network is transmitted to the problem through the Lagrange multiplier λ
  - ✓ we can still capture the overall behavior of the material when the network changes
  - ✓ the network may be defined via one-dimensional models
  - ✓ the network may be patient specific, and overlapped with a fixed background grid

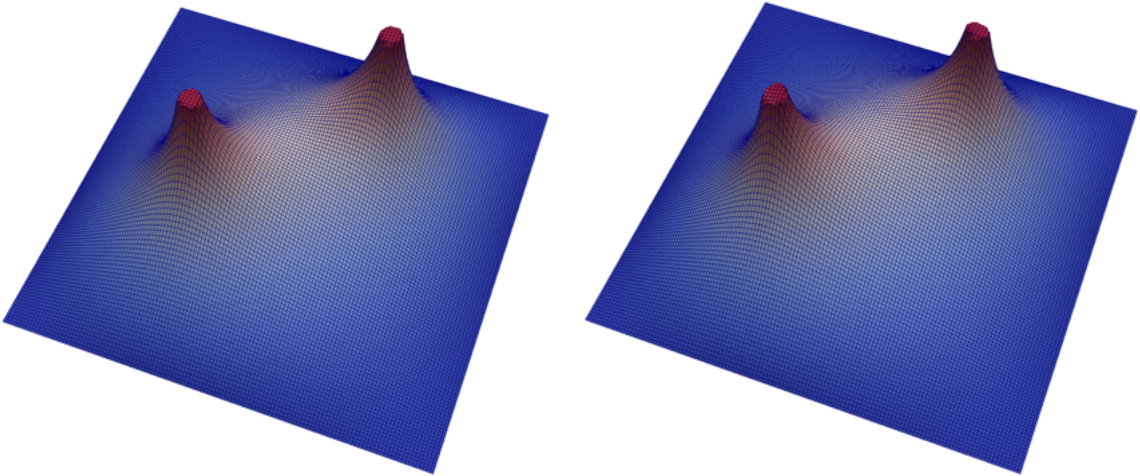
Simple example of restriction operator

Comparison with two vessels: Lagrange multiplier (left) and reduced Lagrange multiplier (right) – $\varepsilon = .2$



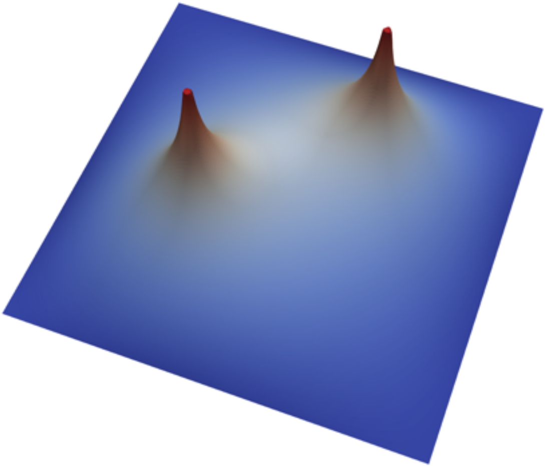
Simple example of restriction operator

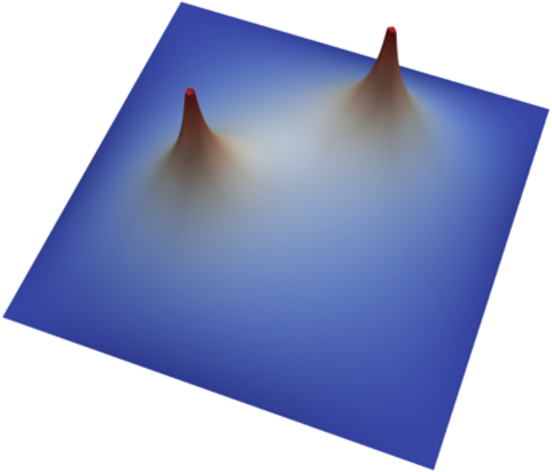
Comparison with two vessels: Lagrange multiplier (left) and reduced Lagrange multiplier (right) – $\varepsilon = .05$



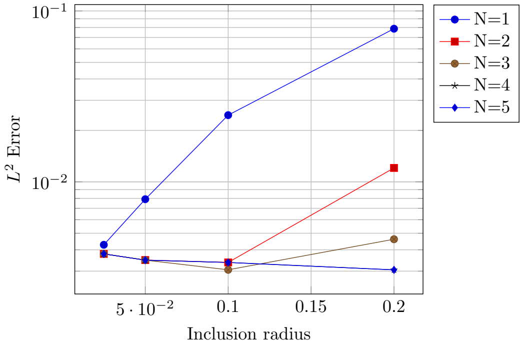
Simple example of restriction operator

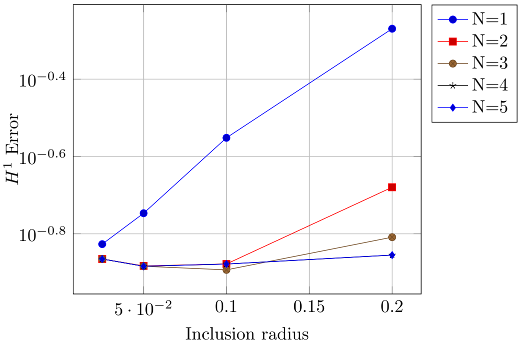
Comparison with two vessels: Lagrange multiplier (left) and reduced Lagrange multiplier (right) – $\varepsilon = .02$





Error with respect to inclusion size

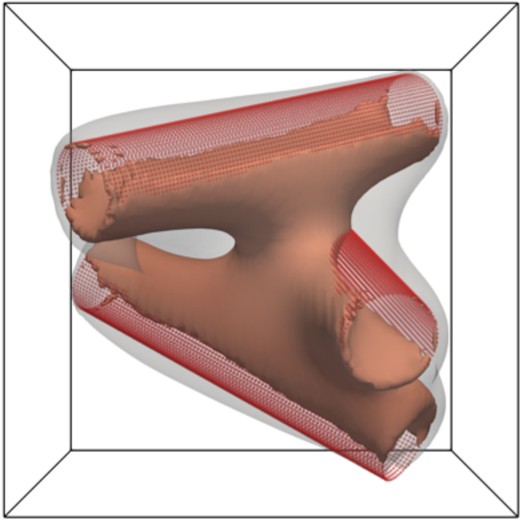


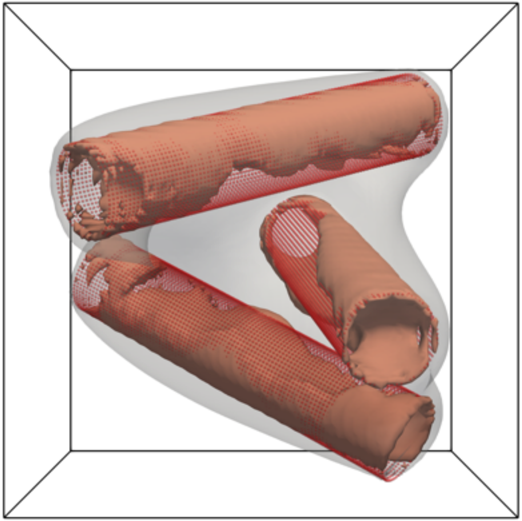


Bottom line: when the inclusion size is small **or** the number of modes is large, the error is comparable to the finite element approximation error (i.e., the error computed with a **full** Lagrange multiplier method, that is, a Fictitious domain method on the **full** inclusion domain)

Comparison between one Fourier mode and three Fourier modes

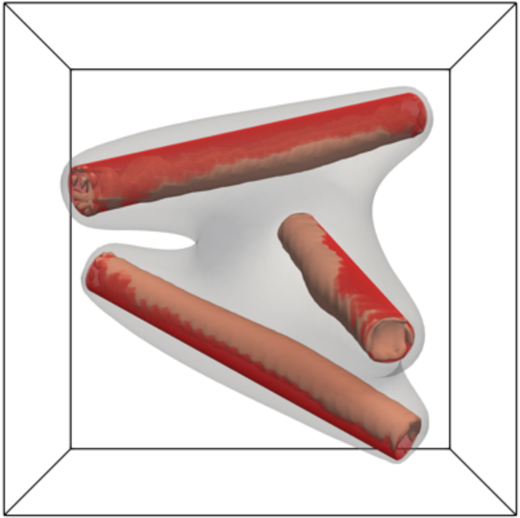
Impose constant value on the surface of three cylinders with radius $r = 0.2$

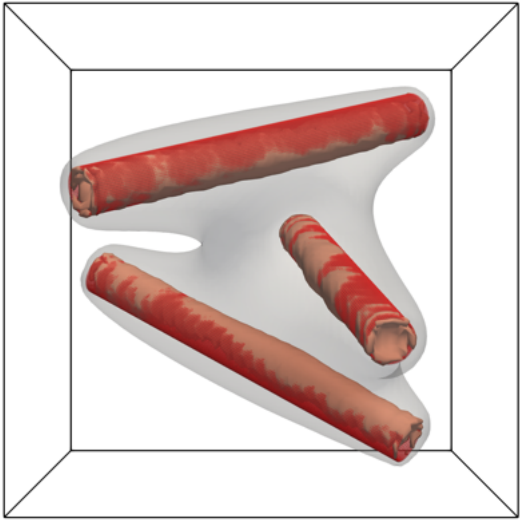




Comparison between one Fourier mode and three Fourier modes

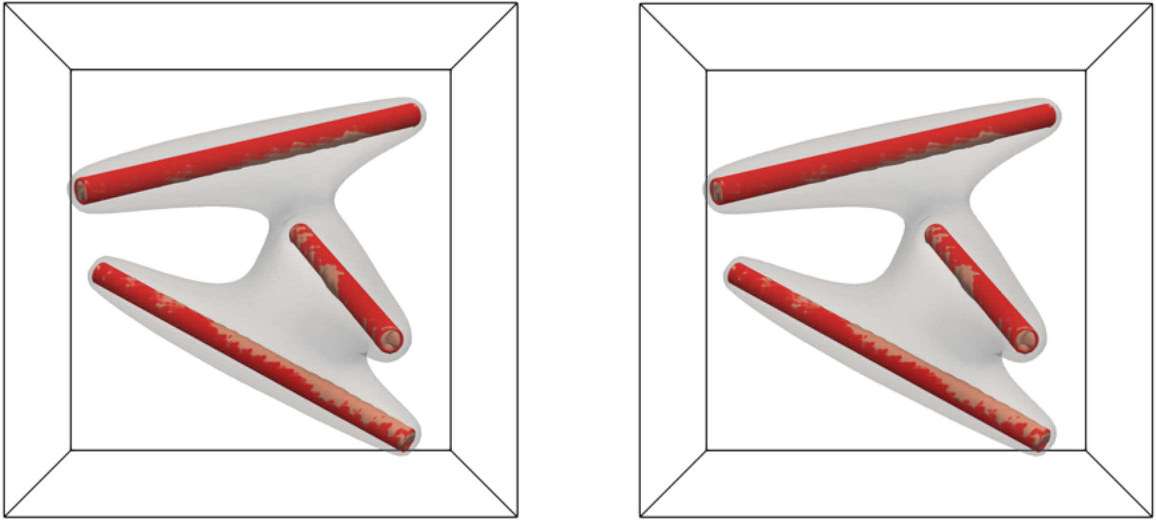
Impose constant value on the surface of three cylinders with radius $r = 0.1$





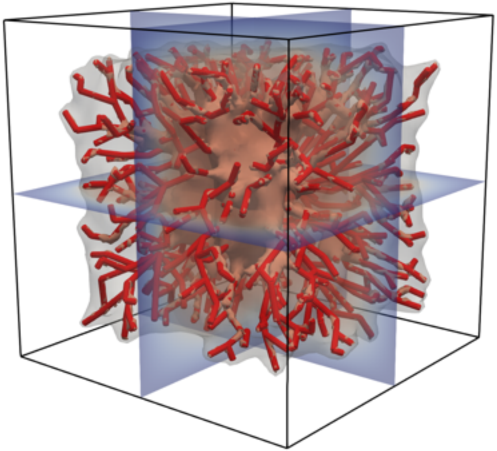
Comparison between one Fourier mode and three Fourier modes

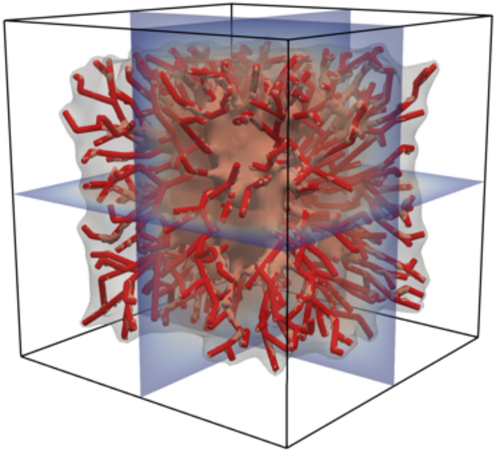
Impose constant value on the surface of three cylinders with radius $r = 0.05$



Comparison between one Fourier mode and three Fourier modes

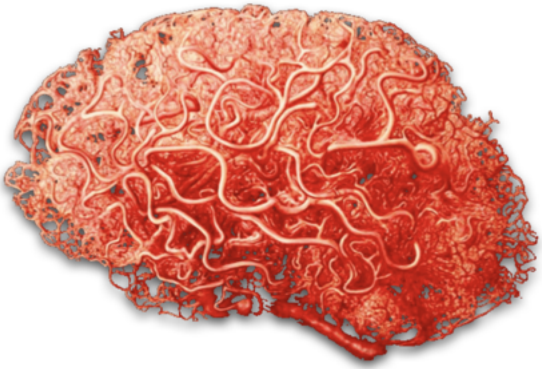
Impose constant value on the surface of complex network with small vessels





Vascularized tissue

Grey matter +



Vasculature

Application to vascularized tissue (reduced FSI)

- Model a bi-phasic tissue, *separately*
  - elastic matrix
  - thin fluid vasculature

Main assumptions

- elastic matrix, approximated variationally using Finite Elements
- the radius of the fluid vessels is much smaller than the size of the characteristic domain
- the fluid vasculature are approximated by one-dimensional manifolds
- the effect of the 1D fluid and of the 1D fibers is included in the 3D elasticity equations by means of (hyper) singular source terms
- The discretization of the grids for the elastic matrix, and fluid vasculature are independent (but the problems are fully coupled!)

Asymptotic formulation – Eliminating the Lagrange multiplier

From fully coupled problem...

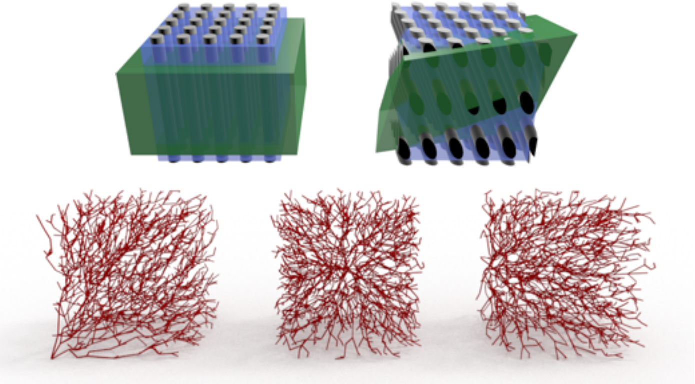
$$
\begin{aligned}
\mathscr{A} u & & +\mathscr{C}^T\lambda &= F & \text{in } V' \\
& (\mathscr{K} - \mathscr{A}_B) w & -\mathscr{M}^T\lambda &= 0 & \text{in } W' \\
\mathscr{C} u & -\mathscr{M} w & &= 0 & \text{in } Q'
\end{aligned}
$$

- ✓ Compute some expansion of λ in terms of w and u (say $\lambda \sim \mathscr{E}(w,u)$)
- ✓ use expansion in the coupling

...to asymptotically coupled problem:

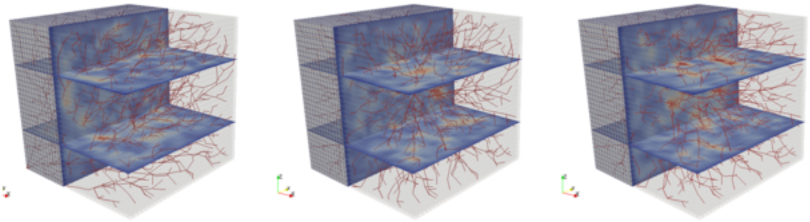
$$
\begin{aligned}
\mathscr{A}_\Omega u & & +\mathscr{C}^T\mathscr{E}(w,u) &= F & \text{in } V' \\
& (\mathscr{K} - \mathscr{A}_B) w & -\mathscr{M}^T\mathscr{E}(w,u) &= 0 & \text{in } W'
\end{aligned}
$$

Constant pressure model



LH and Alfonso Caiazzo. Multiscale modeling of vascularized tissues via non-matching immersed methods. *International Journal for Numerical Methods in Biomedical Engineering*, 35(12):e3264, 2019

Could explain discrepancy between *In Vivo* (MRE) and *In Vitro* (Indendation) experimental observations



LL

$$\begin{pmatrix} -3.00e-03 & 3.30e-04 & 2.00e-04 \\ 3.04e-04 & -2.84e-03 & 4.07e-04 \\ 2.05e-04 & 2.12e-04 & -2.60e-03 \end{pmatrix}$$

C

$$\begin{pmatrix} -5.06e-03 & -1.33e-04 & 7.93e-07 \\ 1.28e-04 & -5.05e-03 & -6.61e-05 \\ 6.16e-05 & -7.52e-05 & -5.43e-03 \end{pmatrix}$$

FC

$$\begin{pmatrix} -1.11e-03 & 4.52e-06 & 6.23e-05 \\ 5.76e-05 & -4.61e-03 & 1.71e-05 \\ 2.25e-05 & -5.25e-05 & -4.29e-03 \end{pmatrix}$$

- ✓ estimate, in silico, shear and compression effects due to the presence of pressurised vessel networks
- ✓ pressure in the (microscopic) vasculature induces a (macroscopic) shear
- ✓ pressure induced shear is highly correlated with the orientation of the underlying vasculature

One-dimensional blood flow model

- Cross-sectional area $A(s,t)$
- Mass flow rate $q(s,t)$
- Average blood pressure over the cross section $p(s,t)$
- One-way coupling with elasticity problem

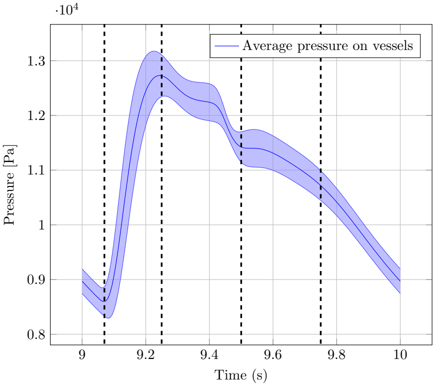
Blood flow in one dimensional networks

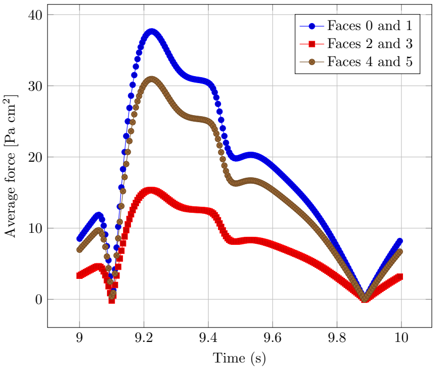
$$\begin{cases} \dfrac{\partial A}{\partial t} + \dfrac{\partial q}{\partial s} = 0, \\ \dfrac{\partial q}{\partial t} + \dfrac{\partial}{\partial s}\left(\dfrac{q^2}{A}\right) + \dfrac{A}{\rho}\dfrac{\partial p}{\partial s} = -\dfrac{8\pi\eta}{\rho}\dfrac{q}{A}. \end{cases}$$

L. O. Müller and P. J. Blanco. A high order approximation of hyperbolic conservation laws in networks: Application to one-dimensional blood flow .
Journal of Computational Physics, 300:423–437, 2015

Coupled physiological pressure model

Average blood vasculature effect on tissue sample walls

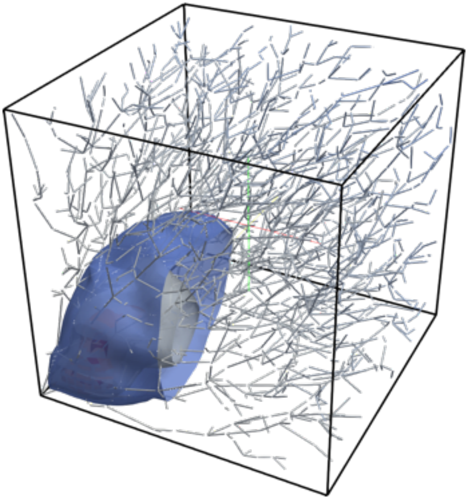




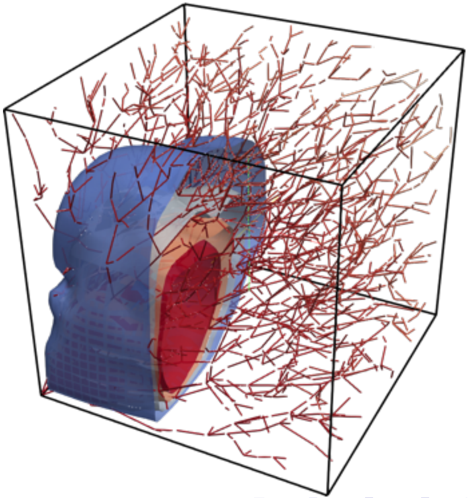
LH, Alfonso Caiazzo, and Lucas Müeller. Multiscale coupling of one-dimensional vascular models and elastic tissues. *Annals of Biomedical Engineering*, 2021

Blood vasculature effect on internal tissue pressure - I

t=9.075 s

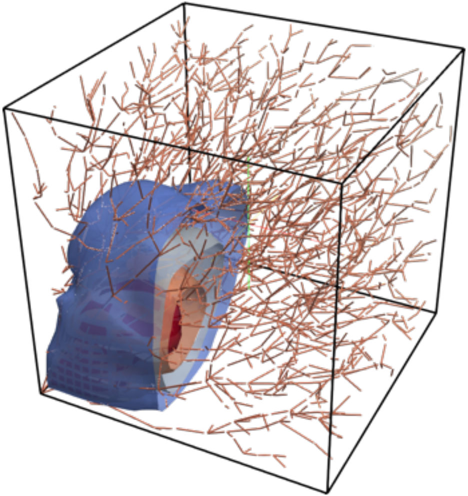


t=9.25 s

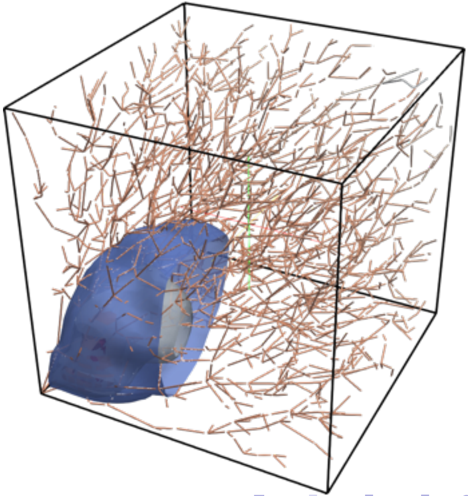


Blood vasculature effect on internal tissue pressure - II

t = 9.5 s



t = 9.75 s



Conclusions

- ✓ Reduced Lagrange multipliers offer a very nice theoretical framework the study of multi-dimensional coupling
- ✓ Both one-way and two-way coupling follow naturally, resulting in a saddle-point structure
- ✓ 3D-1D coupling allows to bridge the gap between fully resolved simulations and homogenized approach, offering a valid (and cheap!) intermediate regime for meso-scale resolutions

References

LH and Paolo Zunino. Reduced lagrange multiplier approach for non-matching coupling of mixed-dimensional domains, 2023.
Submitted

LH, Alfonso Caiazzo, and Lucas Müeller. Multiscale coupling of one-dimensional vascular models and elastic tissues.
Annals of Biomedical Engineering, 2021

LH and Alfonso Caiazzo. Multiscale modeling of vascularized tissues via non-matching immersed methods.
International Journal for Numerical Methods in Biomedical Engineering, 35(12):e3264, 2019

Giovanni Alzetta and LH. Multiscale modeling of fiber reinforced materials via non-matching immersed methods.
Computers & Structures, 239:106334, October 2020

LH and Wenyu Lei. A priori error estimates of regularized elliptic problems.
Numerische Mathematik, 146:571–596, 2020

LH and Nella Rotundo. Error estimates in weighted sobolev norms for finite element immersed interface methods.
Computers and Mathematics with Applications, 2019

Thanks to deal.II and to new and old friends!