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An inverse problem in fluid mechanics applied in biomedicine

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One of the main causes of problems in the human cardiovascular system is malformations in the aortic valve. There exist exploratory techniques to verify the status of an aortic valve, but these procedures are invasive. Also, magnetic resonance imaging (MRI) is not able to detect the valve geometry because the dimension of a voxel is greater than the thickness of the valve (between 0.5 and 0.8 mm). Using the perturbed version of the Navier-Stokes equations, a penalization parameter method for obstacle identification in an incompressible fluid flow is presented. The proposed method consists of adding a permeability term to the system such that some subset of its boundary support represents the obstacle, considering the maximum velocity on the inflow as unknown with a known velocity profile, and the use of backflow stabilization given by directional do-nothing condition (DDN) on the outflow. This allows to work in a fixed domain and to highly simplify the solution of the inverse problem via some suitable cost functional.

Substituting obstacles and domain deformations for a permeability term

From the steady Stokes and Navier-Stokes models, a penalization method has been considered by several authors for approximating those fluid equations around obstacles. In order to model our problem, we use fictitious domains to study obstacles immersed in incompressible viscous fluids through a simplified version of Brinkman's law for porous media. If the scalar function γ is considered as the reciprocal of the permeability, it is possible to study the singularities of γ as approximations of obstacles (when γ tends to $+\infty$) or of the domain corresponding to the fluid (when $\gamma = 0$ or is very close to 0). The strong convergence of the solution of the perturbed problem to the solution of the strong problem is studied, also considering error estimates that depend on the penalty parameter, both for fluids modeled with the Stokes and Navier-Stokes equations with inhomogeneous boundary conditions.

In order to validate this theory numerically, a straightforward benchmark is proposed considering a 2D domain containing an immersed obstacle and a domain deformation. This real domain is later transformed into a virtual domain where the obstacle and deformation are modeled in a permeability coefficient. The coefficient γ is set to 0 in the real domain and is equal to a positive constant R in the remainder of the domain. As R increases, the velocity obtained in the virtual domain becomes a better approximation of the velocity in the real domain in accordance with the theory. However, when using FEM with Taylor-Hood elements, the numerical result significantly exceeds the theoretical estimate obtained (see Aguayo and Carrillo, 2022).

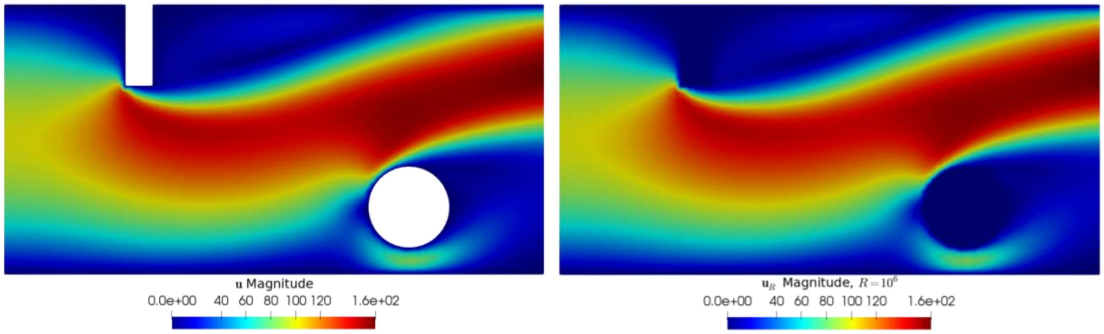

Figure 1: Velocity magnitude in real and virtual domains (from left to right) using FEM with Taylor-Hood elements, $R = 10^6$.

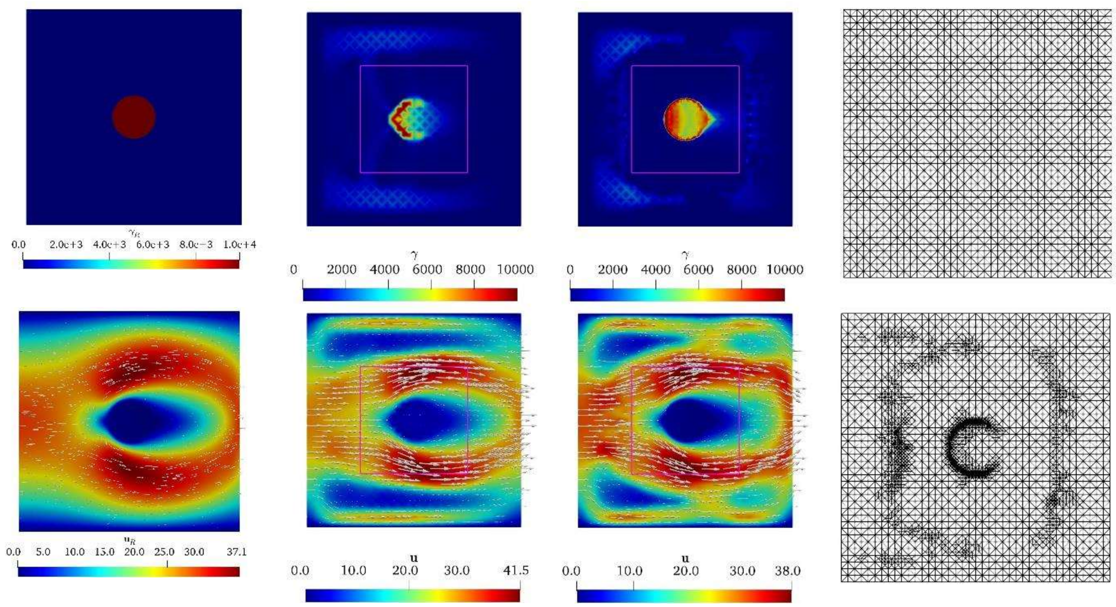

Figure 2: Permeabilities and velocity fields (column 1: references, column 2: optimum before refinement, column 3: optimum after 12 refinement stages). The measurement region is delimited by a rectangle with magenta lines. Column 4 shows the evolution of the mesh refinement (top: original mesh, bottom: refined mesh after 12 stages).

A result of stability for the inverse problem

From a mathematical perspective, the direct problem for the Navier-Stokes equations involves calculating the velocity and pressure of a fluid based on various parameters, including the domain, boundary conditions, viscosity, permeability, and other relevant factors. Our inverse problem involves reconstructing the shape of obstacles or domain deformations based on internal partial velocity measurements of a fluid. Given the knowledge of the domain structure, we aim to determine a permeability coefficient γ that represents the obstacles. While there are results indicating that small disturbances in the permeability coefficient result in proportional disturbances in velocity, the inverse problem requires certain theoretical assumptions to ensure a logarithmic inequality that supports stability in the reconstruction process (see Aguayo and Osses, 2022). Our result is applicable when γ is weakly differentiable from partial measurements of velocity and vorticity field, but it is insufficient when the desired coefficient is discontinuous from a theoretical perspective. However, a numerical test using FEM and adaptive refinement has shown promise in reconstructing a discontinuous coefficient that represents a circular obstacle immersed in the fluid from velocity field measurements within a small subdomain.

A parameter identification problem applied in valve geometry reconstruction

Consider a virtual domain Ω whose boundary $\partial\Omega$ is divided into three disjoint sets Γ_W, Γ_I y Γ_O. These parts represent the no-slip, inflow and outflow boundary conditions, respectively. If $\boldsymbol{u}_R$ denotes the velocity of the fluid being measured and the set ω denotes the velocity measurement region, where $\omega \subseteq \Omega$, we define a new minimization problem with a suitable smooth functional J

$$
\begin{aligned}
&\text{minimize } J(\gamma,\beta) = \frac{1}{2}\|\boldsymbol{u}-\boldsymbol{u}_R\|_{0,\omega}^2 + \frac{\alpha}{2}\|\gamma\|_{1,\Omega}^2 \\
&\text{subject to} \qquad -\nu\Delta\boldsymbol{u} + (\nabla\boldsymbol{u})\boldsymbol{u} + \nabla p + \gamma\boldsymbol{u} = \boldsymbol{0} \quad \text{in } \Omega \\
&\qquad\qquad\qquad \operatorname{div}\boldsymbol{u} = 0 \quad \text{in } \Omega \\
&\qquad\qquad\qquad \boldsymbol{u} = \boldsymbol{0} \quad \text{on } \Gamma_W \\
&\qquad\qquad\qquad \boldsymbol{u} = \beta\boldsymbol{u}_I \quad \text{on } \Gamma_I \\
&\qquad -\nu\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{n}} + p\boldsymbol{n} + \frac{1}{2}(\boldsymbol{u}\cdot\boldsymbol{n})_{-}\boldsymbol{u} = \boldsymbol{0} \quad \text{on } \Gamma_O \\
&\qquad\qquad\qquad 0 \le \gamma \le M_1 \\
&\qquad\qquad\qquad 0 \le \beta \le M_2
\end{aligned}
$$

where $\|\boldsymbol{u}-\boldsymbol{u}_R\|_{0,\omega}^2 = \int_\omega |\boldsymbol{u}-\boldsymbol{u}_R|^2\,d\boldsymbol{x}$, $\|\gamma\|_{1,\Omega}^2 = \int_\Omega (|\gamma|^2 + |\nabla\gamma|^2)\,d\boldsymbol{x}$, $\boldsymbol{n}$ is the outer normal vector, $\boldsymbol{g}$ is a preset inflow profile, α, M_1 and M_2 are positive constants.

The cost functional J depends on the parameters γ and β, since the velocity of the fluid depends on both. In this case, the term $\frac{\alpha}{2}\|\gamma\|_{1,\Omega}^2$ corresponds to a Tikhonov regularization that helps the problem to be solved more easily from a numerical perspective. As the constant α is smaller, the parameters will be better adjusted to the velocity $\boldsymbol{u}_R$. However, if this measurement has a considerable amount of noise or if its resolution is low, it is necessary to use a larger α parameter to avoid overfitting. In addition, the fact of not measuring the vorticity makes it imperative that a regularizing term be added. Existence of local minimizers and first and second order optimality conditions are derived through the differentiability of the solutions of the Navier-Stokes equations, including the directional do-nothing condition, with respect to γ and β (see Aguayo et al,, 2020).

Several numerical experiments implemented in FEniCS (with dolfin-adjoint library) illustrate the applicability of the method, for the localization of a 2D and 3D cardiac valve from MRI flow type imaging data (see Aguayo, 2022). The numerical results for the 2D case are presented in Figure 3. We draw a magenta polyline that follows the points where the optimal state γ^* reaches its maximum values on each side of the axis of symmetry, which closely approximate the inner border of the valves. The optimum γ^* assumes values close to 0 between the valves, above and below them, as expected.

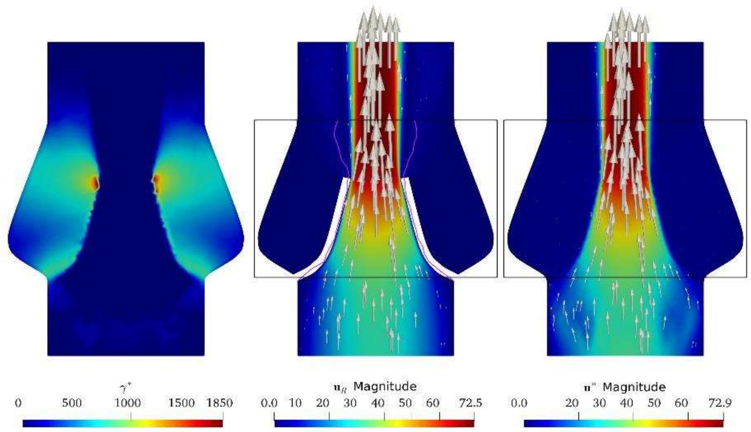

Figure 3. Optimal γ^*, reference solution $\boldsymbol{u}_R$ with reconstructed valve and optimal velocity $\boldsymbol{u}^*$ (from left to right). 2D Test, 366 iterations with L-BFGS-B. The measurement region is delimited by a rectangle with black lines (see Aguayo, 2022).

The 3D experiment is based on a parameterized valve, where the reference is transformed by projecting the velocity $\boldsymbol{u}_\mathrm{R}$ into the piecewise constant function space on a hexahedral mesh in order to simulate a 4D Flow MRI. It can be seen that the optimum γ^* assumes values close to 0 in areas before and after the valve, as well as in the area between the valves. Choosing the region where γ^* has values greater or equal than $0.4\max\{\gamma^*(\boldsymbol{x}) \mid \boldsymbol{x} \in \Omega\}$, following a threshold criterion to identify the valve, it can be seen that region delimits the space between the valves. The magnitude and direction of $\boldsymbol{u}^*$ and $\boldsymbol{u}_\mathrm{R}$ are similar.

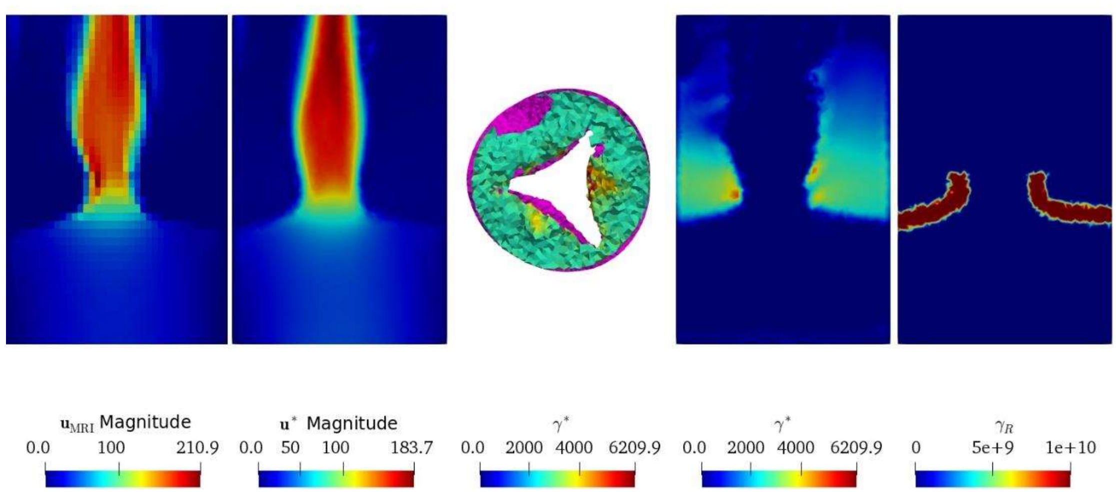

Figure 4. Isovalues cuts. Simulated MRI $\boldsymbol{u}_R$, $\boldsymbol{u}^*$, comparison between γ_R (magenta) and γ^*, γ^* and γ_R (from left to right). 3D MRI Test, 566 iterations (see Aguayo, 2022).

Conclusion and outlook

We have presented an inverse problem focused on recovering the coefficient of permeability in the Stokes and Navier-Stokes equations, with the goal of detecting obstacles and domain deformations.

Our research provides theoretical and numerical validation for using virtual domains and permeability functions to solve this inverse problem, with successful recovery of patency functions and valve shapes, although with some limitations due to numerical noise and running time. As the 3D model is particularly relevant to the medical community as a diagnostic tool for valvular conditions, our future work includes designing an improved and simplified version of our numerical algorithm.

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