Domain Decomposition Solvers for Operators with Fractional Interface Perturbations

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1 Introduction

Mathematical models featuring interaction of physical systems across a common interface describe numerous phenomena in engineering, environmental sciences and medicine. Here the large variations in material coefficients or wide ranges of temporal/spatial scales at which the phenomena can be studied demand parameter-robust solution algorithms. In [3, 4] such algorithms were recently developed for Darcy-Stokes and Biot-Stokes models by establishing uniform stability of the respective problems in (non-standard) parameter-dependent norms. In particular, the authors show that in order to attain robustness, mass conservation at the interface Γ of the porous domain Ω must be accounted for in the functional setting, leading to control of the porous pressure p in the norm $\|p\|_\Omega$ such that

$$\|p\|^2_\Omega = \|K^{1/2}\nabla p\|^2_{0,\Omega} + \|\mu^{-1/2} p\|^2_{-1/2,\Gamma}. \tag{1}$$

Here $\|\cdot\|_{k,D}$ denotes the standard norm of Sobolev space $H^k(D)$ on domain D. The coefficients $K, \mu > 0$ are due to material properties, namely the permeability of the porous medium and the fluid viscosity.

By operator preconditioning, the choice of norm (1) yields a Riesz map preconditioner $b \mapsto x$ defined by solving the problem

$$-K\Delta_\Omega x + \mu^{-1}(-\Delta_\Gamma)^{-1/2} x = b. \tag{2}$$

Note that the operator in (2) contains a bulk part $-\Delta_\Omega$ and an interface part $(-\Delta_\Gamma)^{-1/2}$, which, from the point of view topological dimension of the underlying domains, can be viewed as a lower order *perturbation*.

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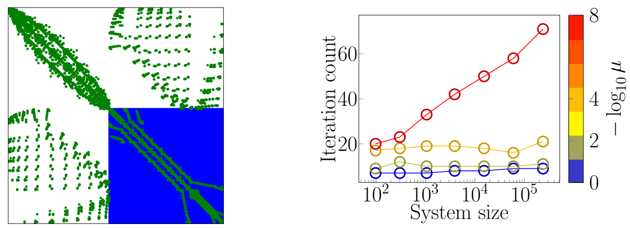

Fig. 1 (Left) Sparsity pattern of the operator in (2) on $\Omega = (0,1)^3$ with $\Gamma \subset \partial\Omega$. Interface perturbation leads to dense block (in blue) which is challenging for sparse LU solvers. (Right) Number of PCG iterations under mesh refinement when solving (2) on $\Omega = (0,1)^2$ with $\Gamma \subset \partial\Omega$ and AMG [8] preconditioner. In both case case $K = 1$ and the problems are discretized by continuous linear Lagrange ($\mathbb{P}_1$) elements.

Efficiency of the block-diagonal Darcy/Biot-Stokes preconditioners [3, 4] hinges on performant solvers for (2). However, the problem might not be amenable to standard (generic, black-box) approaches especially in case when the fractional interface perturbation becomes dominant. We illustrate this behavior in Figure 1 where (2) is solved by preconditioned conjugate gradient (PCG) method with algebraic multigrid (AMG) preconditioner. Indeed, the number of iterations increases with the weight of the perturbation term and, worryingly, for large enough values mesh-independence is lost.

Non-overlapping domain decomposition (DD) is a solution methodology which has been successfully applied to number of challenging problems including coupled multiphysics systems e.g. [5, 7, 11]. A key component of the method are then the algorithms for the problems arising at the interface which can be broadly divided into two categories. In FETI or BDDC variants (see e.g. [1] and references therein) the solvers utilize suitable auxiliary problems on the *subdomains*. To develop tailored solvers for operators with fractional interface perturbation we here follow an alternative approach [1] and address the problem directly at the *interface*. In particular, we shall construct preconditioners for the resulting Steklov-Poincaré operators using sums of fractional order interfacial operators which include contribution due to the DD and the perturbation (which is only localized at the interface).

2 Domain decomposition solvers

We shall consider solvers for (2) in a more general setting. To this end, let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ be a bounded domain with Lipschitz boundary $\partial\Omega$, and $\Gamma \subseteq \partial\Omega$. Moreover, let $V = V(\Omega)$, $Q = Q(\Gamma)$ be a pair of Hilbert spaces with V', Q' being their respective duals and let $R\colon V \to Q'$ be a restriction operator. For $b \in V'$ we are then interested in solving

$$\mathcal{A}x = b \text{ in } V' \quad \text{with} \quad \mathcal{A} = A_\Omega + \gamma R' B_\Gamma^{-1} R, \tag{3}$$

where $\gamma \geq 0$ and $A_\Omega\colon V \to V'$ is some symmetric operator coercive on V while $B_\Gamma\colon Q \to Q'$ is assumed to induce an inner product on Q. Note that the norm operator in (2) is a special case of (3) with $V = H^1_0(\Omega)$, $Q = H^{1/2}(\Gamma)$, R the trace operator and $A_\Omega = -K\Delta_\Omega$ while $B_\Gamma = (-\Delta_\Gamma)^{1/2}$.

To formulate our non-overlapping domain decomposition approach for (3), we follow [1] and decompose $V = V_0 \oplus V_\Gamma$ where $V_0 = \{v \in V; Rv = 0\}$. Assuming that V_Γ can be identified with Q we observe that the operator $\mathcal{A}$ takes a block structure

$$\mathcal{A} = \left(\begin{array}{c|c} A^{00}_\Omega & A^{0i}_\Omega \\ \hline A^{i0}_\Omega & A^{ii}_\Omega \end{array}\right) + \gamma \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \tilde{B}^{-1}_\Gamma \end{array}\right), \tag{4}$$

which we exploit to design a preconditioner for $\mathcal{A}$. Specifically, under the assumption that A^{00}_Ω is invertible, let us define the DD preconditioner

$$\mathcal{B} = \left(\begin{array}{c|c} I^{00}_\Omega & -(A^{00}_\Omega)^{-1}A^{0i}_\Omega \\ \hline 0 & I^{ii}_\Omega \end{array}\right) \left(\begin{array}{c|c} A^{00}_\Omega & 0 \\ \hline 0 & S_\Gamma \end{array}\right)^{-1} \left(\begin{array}{c|c} I^{00}_\Omega & 0 \\ \hline -A^{i0}_\Omega(A^{00}_\Omega)^{-1} & I^{ii}_\Omega \end{array}\right). \tag{5}$$

Here $I^{00}_\Omega\colon V_0 \to V_0$ and $I^{ii}_\Omega\colon V_\Gamma \to V_\Gamma$ are identity operators on the respective subspaces while S_Γ is spectrally equivalent to the DD Schur complement/Steklov-Poincaré operator $S^*_\Gamma = A^{i0}_\Omega(A^{00}_\Omega)^{-1}A^{0i}_\Omega + A^{ii}_\Omega + \gamma\tilde{B}^{-1}_\Gamma$. We note that preconditioner (5) preserves symmetry of the original problem (3) as we target PCG solvers. However, with Krylov methods which do not require symmetry a more efficient triangular variant of the preconditioner is sufficient.

Our main contribution is an observation that for problems with interface perturbations, the Schur complement approximation S_Γ in (5) takes the form

$$S_\Gamma = L^s_A + \gamma L^t_B, \tag{6}$$

for some constants $s, t \in \mathbb{R}$ and symmetric, positive-definite operators L_A, L_B depending on the regularity of $\mathcal{A}$, the restriction operator and the perturbation. In particular, the structure of the preconditioner reflects the two contributions to the Schur complement; the decomposition $V = V_0 \oplus V_\Gamma$ applied to operator A_Ω yields L^s_A while L^t_B is due to the perturbation.

Motivated by the initial example (2) we shall in the following focus on problems for which $-1 < s, t < 1$ and L_A, L_B are spectrally equivalent to $L = -\Delta_\Gamma + I_\Gamma$. However, we highlight that the operators might in general differ by their boundary conditions (which for L_A reflect boundary conditions on $\partial\Omega \setminus \Gamma$ imposed on V in (3)).

Assuming that $(A^{00}_\Omega)^{-1}$ can be efficiently computed, the main challenge for scalability of preconditioner (5) is an efficient realization of (an approximate) inverse of (6). Upon discretization, the operators L^s_A, L^t_B can be approximated by eigenvalue factorization[1]. However, this approach suffers from cubic scaling. For the specific case of $L^{1/2}$ a more efficient strategy with improved scaling is applied in [1] based on the Lanczos process while, more recently, [9] proves that rational approximations (RA) lead to non-overlapping DD methods with linear scaling. Building on this observation to obtain order optimal solvers for the perturbed problem (3) we follow [6] where rational approximations[2] were developed for Riesz maps with norms induced by sum operator $\alpha L^s + \beta L^t$ with $\alpha, \beta \geq 0$. In particular, this setting fits our Schur complement operator (6) if constant material properties *and* suitable boundary conditions are prescribed on $\mathcal{A}$ in (3).

3 Model problem

We shall illustrate performance of the domain decomposition preconditioner (5) using a model interface-perturbed problem: Find $x \in V = H^1(\Omega)$ such that

$$K(-\Delta_\Omega + I_\Omega)x + \gamma(-\Delta_\Gamma + I_\Gamma)^t x = b \text{ in } V', \tag{9}$$

where $K > 0$, $\gamma \geq 0$ and $-1 < t < 1$. Here $\Omega = (0,1)^d$, $d = 2, 3$ and $\Gamma = \partial\Omega$. We note that this choice maximizes the size of the interface. At the same times, it enables the RA-favorable setting of $L_A = L$, $L_B = L$, $L = -\Delta_\Gamma + I_\Gamma$ in (6). Following [1] the DD Schur complement of the operator $A_\Omega = K(-\Delta_\Omega + I_\Omega)$ in (3) is spectrally equivalent to fractional operator $KL^{1/2}$. In turn we apply preconditioner (5) with $S_\Gamma = KL^{1/2} + \gamma L^t$. However, for simplicity, we shall fix K, here $K = 3$, and we only investigate the effect of perturbation strength.

In the numerical experiments we consider H^1-conforming finite element spaces $V_h \subset V$ constructed in terms of $\mathbb{P}_1$ elements. Consequently, the matrix realization

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[1] For $L\colon Q \to Q'$ let L_h be the matrix realization of the operator in the basis of some finite dimensional approximation space Q_h, $n = \dim Q_h$. Moreover, let M_h be the mass matrix, i.e. matrix realization of the inner product of the Lebesgue space L^2 on Q_h. Assuming L is symmetric and positive definite, the factorization $L_h U_h = M_h U_h \Lambda_h$, $U_h^T M_h U_h = \mathrm{Id}$ holds where Λ_h is a diagonal matrix of eigenvalues while the corresponding eigenvectors constitute the columns of matrix U_h. We then define

$$L_h^s = (M_h U_h)\Lambda_h^s (M_h U_h)^T. \tag{7}$$

Note that for $L = (-\Delta + I)$ and $f \in Q$ represented in Q_h by interpolant with coefficient vector $f_h \in \mathbb{R}^n$ the function $f_h \mapsto f_h \cdot L_h^s f_h$ represents an approximation of the square of the Sobolev norm $\|f\|_s^2$.

[2] Referring to the definitions in (7) the RA construct approximate solutions $x \in Q$ satisfying $\alpha L^s x + \beta L^t x = b$, $b \in Q'$ in the finite dimensional space Q_h via a solution operator

$$c_0 M_h^{-1} + \sum_{k=1}^{m} c_i (L_h + p_k M_h)^{-1}. \tag{8}$$

Here, $c_i \in \mathbb{R}$ and $p_i \geq 0$ are respectively the residues and the poles of the rational approximation f_{RA} to function $f : x \to (\alpha x^s + \beta x^t)^{-1}$. Importantly, the number of poles m does not depend on the dimensionality of Q_h and is instead determined by the accuracy ϵ_{RA} of the RA, i.e. $\|f - f_{\mathrm{RA}}\| \leq \epsilon_{\mathrm{RA}}$. We refer to [6, 9] and references therein for more details.

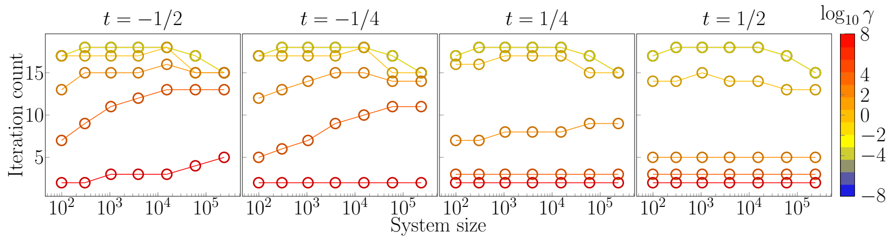

Fig. 2 PCG iterations when solving (9) on $\Omega = (0,1)^2$ and preconditioner (5) with $S_\Gamma = KL^{1/2} + \gamma L^t$. Problem is discretized by $\mathbb{P}_1$ elements. Blocks of the preconditioner are here computed exactly.

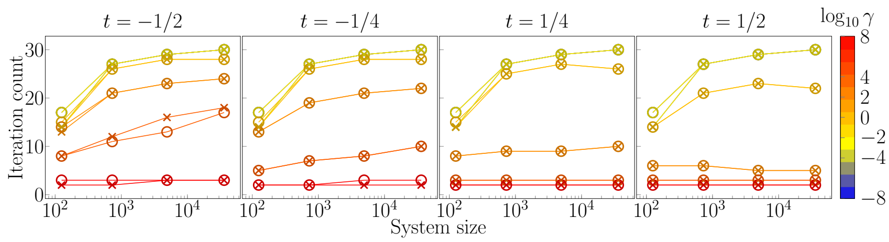

Fig. 3 PCG iterations when solving (9) on $\Omega = (0,1)^3$ and preconditioner (5) with $S_\Gamma = KL^{1/2} + \gamma L^t$. Problem is discretized by $\mathbb{P}_1$ elements. Leading block of preconditioner is computed exactly. Results with realization of the Schur complement preconditioner by RA with tolerance $\epsilon_{\mathrm{RA}} = 10^{-14}$ are depicted by (○) markers while (×) markers correspond to definition via the eigenvalue problem (7).

of the fractional interface perturbation reads $\gamma T_h^T L_h^t T_h$ where matrix L_h^t is defined in (7) and T_h is a discrete trace operator such that $T_h\phi = \sum_{j=1}^{n} l_j(\phi|_\Gamma)\psi_j$ for any $\phi \in V_h$ and $\psi_j, l_j, j = 1,\cdots,n$ being respectively the basis functions and degrees of freedom (point evaluations) of the discrete trace space $V_{\Gamma,h} = Q_h$ built likewise using $\mathbb{P}_1$ elements.

The linear systems due to discretization of (9) shall be solved by PCG solver using our DD preconditioner (5) which now requires inverse of the linear system due to $KL_h^{1/2} + \gamma L_h^t$. Here we shall either apply the eigenvalue realization (7) (which allows for closed form evaluation of the exact inverse) or the approximate inverse due to RA, see (8). To put focus on the Schur complement action of blocks $(A_\Omega^{00})^{-1}$ in (5), that is, in the diagonal and triangular factors of $\mathcal{B}$, will be computed (exactly) by LU factorization. For results with approximate inverse of A_Ω^{00} we refer to Remark 1. Finally, the PCG solver is always started from 0 initial vector and terminates upon reducing the preconditioned residual norm by factor 10^{10}.

We summarize performance of the DD preconditioner in Figure 2 and Figure 3 which consider (9) with $\Omega = (0,1)^2$ and $\Omega = (0,1)^3$ respectively. It can be seen that the PCG convergence is in general bounded in mesh size, fractionality t and the perturbation strength γ. Important for the scalability of (5) is the observation that iteration counts with RA realization of the Schur complement preconditioner

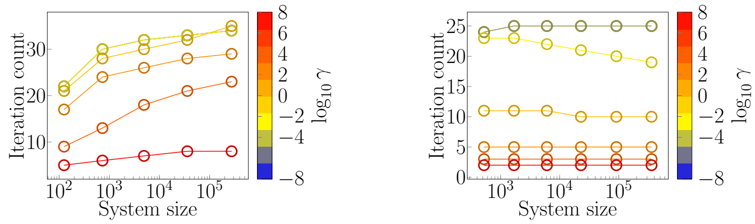

Fig. 4 PCG iterations for computing the inverse of fractional perturbed operators by preconditioner (5). (Left) The operator is (9) with $t = -1/2$ and $\Omega = (0, 1)^3$. The operator $\mathcal{A}$ (4) and the preconditioner are evaluated using RA. On the finest refinement level $\dim V_{\Gamma,h} = 24 \cdot 10^3$. (Right) Operator (10) is considered with $S_\Gamma = K L^{-1/2} + \gamma I_\Gamma$ in the Schur complement (6). In both cases $\Gamma = \partial\Omega$.

practically match the exact inverse of S_Γ. We remark that the chosen tolerance of $\epsilon_{\mathrm{RA}} = 10^{-14}$ yields roughly $m = 20$ poles in (8). The computation setup in $3d$ then leads to linear systems with < 6200 unknowns at the interface.

Remark 1 (Evaluation of the operator in (9)*)*

In numerical experiments shown in Figure 2 and Figure 3 the operator $\mathcal{A}$ in (9) utilized the eigenvalue decomposition (7) for L_h^t. This realization restricts the size of Γ or $\dim Q_h$ that are computationally tractable. However, action of the perturbation can instead be computed via RA leading to evaluation of $\mathcal{A}$ with optimal complexity and enabling large scale problems. In Figure 4 we revisit (9) with $t = -1/2$, $\Omega = (0, 1)^3$ and RA used both for the operator and the preconditioner (5). Moreover, to illustrate performance when the preconditioner blocks are inexact, all instances of $(A_\Omega^{00})^{-1}$ shall here, for simplicity, be approximated by a single V-cycle of AMG [8]. The number of PCG iterations then appears to be bounded in the mesh size and the parameter γ. As before, $\mathbb{P}_1$ elements were used for discretization.

Remark 2 (Application to $\boldsymbol{H}$*(div)-elliptic problem)* Preconditioners (5) are not limited to H^1-elliptic problems. To illustrate this fact we consider $V = \boldsymbol{H}(\mathrm{div}, \Omega)$, $\Omega = (0, 1)^2$ and a variational problem induced by bilinear form due to operator $\mathcal{A}$

$$\langle \mathcal{A}\boldsymbol{u}, \boldsymbol{v}\rangle = \int_\Omega K(\boldsymbol{u} \cdot \boldsymbol{v} + \nabla \cdot \boldsymbol{u} \nabla \cdot \boldsymbol{v}) + \gamma \int_{\partial\Omega} \boldsymbol{u} \cdot \boldsymbol{\nu} \boldsymbol{v} \cdot \boldsymbol{\nu} \quad \forall \boldsymbol{u}, \boldsymbol{v} \in V. \qquad (10)$$

We observe that $\mathcal{A}$ falls under the template problem (3). In order to apply the domain-decomposition preconditioner we then require a preconditioner for the DD Schur complement due to $(A_\Omega^{00})^{-1}$ where A_Ω^{00} is here the operator $K(I - \nabla\nabla\cdot)$ on $\boldsymbol{H}_0(\mathrm{div}, \Omega)$. Motivated by [2], we shall to this end consider the operator $L_A = KL^{-1/2}$ so that S_Γ in (5) is defined as $S_\Gamma = KL^{-1/2} + \gamma I_\Gamma$. For numerical experiments the system is discretized by lowest order Brezzi-Douglas-Marini elements which lead to the discrete trace space $V_{\Gamma,h} = Q_h$ of discontinuous piecewise-linear functions on trace mesh Γ_h. Robustness of the resulting preconditioner is shown in Figure 4.

4 Darcy-Stokes preconditioning

We finally apply the proposed non-overlapping DD solvers to realize preconditioners for the coupled Darcy-Stokes model with Darcy problem in the primal form [7]. That is, assuming bounded domains $\Omega_S, \Omega_D \subset \mathbb{R}^d$, $d = 2, 3$ sharing a common interface Γ (cf. Figure 5) we seek to find the Stokes velocity $\boldsymbol{u}_S$, the Stokes pressure p_S and the Darcy pressure p_D such that

$$\begin{aligned} -\nabla\cdot\sigma(\boldsymbol{u}_S, p_S) = \boldsymbol{f}_S \text{ and } \nabla\cdot\boldsymbol{u}_S = 0 &\qquad \text{in } \Omega_S,\\ -\nabla\cdot K\nabla p_D = f_D &\qquad \text{in } \Omega_D,\\ \boldsymbol{u}_S\cdot\boldsymbol{\nu} + K\nabla p_D\cdot\boldsymbol{\nu} = 0 &\qquad \text{on } \Gamma,\\ -\boldsymbol{\nu}\cdot\sigma(\boldsymbol{u}_S, p_s)\cdot\boldsymbol{\nu} - p_D = 0 &\qquad \text{on } \Gamma,\\ -P_{\boldsymbol{\nu}}\left(\sigma(\boldsymbol{u}_S, p_S)\cdot\boldsymbol{\nu}_S\right) - \alpha\mu K^{-1/2}P_{\boldsymbol{\nu}}\boldsymbol{u}_S = 0 &\qquad \text{on } \Gamma, \end{aligned} \tag{11}$$

where $P_{\boldsymbol{\nu}}$ is the tangential trace operator $P_{\boldsymbol{\nu}}\boldsymbol{u} = \boldsymbol{u} - (\boldsymbol{u}\cdot\boldsymbol{\nu})\boldsymbol{\nu}$ and $\sigma(\boldsymbol{u}, p) = \mu\nabla\boldsymbol{u} - p\mathrm{Id}$. In addition to the previously introduced coefficients K, $\mu > 0$ the model also includes the Beavers-Joseph-Saffman parameter $\alpha \geq 0$. The system (11) is closed by prescribing suitable boundary conditions to be discussed shortly.

We consider (11) with a parameter-robust block diagonal preconditioner [4]

$$\mathcal{B} = \operatorname{diag}\left(-\mu\Delta + \alpha\mu K^{-1/2}P'_{\boldsymbol{\nu}}P_{\boldsymbol{\nu}}, \mu^{-1}I, -K\Delta + \mu^{-1}(-\Delta_\Gamma)^{-1/2}\right)^{-1}. \tag{12}$$

Observe that both the first and the final block in (12) are of the form of the interface-perturbed operators (3). However, for simplicity we shall here set $\alpha = 0$ and only focus on the pressure preconditioner. In particular, to efficiently approximate (2) we shall perform few PCG iterations with the DD preconditioner (5) using $S_\Gamma = KL^{1/2} + \mu^{-1}L^{-1/2}$ in the Schur complement. We note that the interface operator is thus identical to the one utilized in robust preconditioning of mixed Darcy-Stokes model [10].

To illustrate performance of the preconditioner (12) we consider (11) in a $3d$ domain pictured in Figure 5 and set[3] $K = 10^{-2}$, $\mu = 10^{-4}$. Using discretization by $\mathbb{P}_2$-$\mathbb{P}_1$-$\mathbb{P}_2$ elements the linear system is solved by preconditioned Flexible GMRes (FGMRes). The Darcy-Stokes preconditioner is then realized by applying single AMG V-cycle for the Stokes blocks while the Riesz map of the Darcy pressure (2) is approximated by PCG solver using (5) and running with a relative tolerance of 10^{-4}. The DD preconditioner uses RA with tolerance $\epsilon_{\mathrm{RA}} = 10^{-14}$ and AMG for the leading block in (5). With this setup the scalability study summarized in Figure 5 reveals that the proposed solver is order optimal.

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[3] Due to computational demands we did not perform parameter-robustness study for $d = 3$. However, with a $2d$ version of the geometry in Figure 5 we observe that (5) with RA approximation of the Schur complement leads to mesh- and parameter-independent Krylov iterations. In particular, $S_\Gamma = KL^{1/2} + \mu^{-1}L^{-1/2}$ leads to K, μ and h bounded iterations when solving (2) with PCG. We omit these results from our presentation due to spatial limitations.

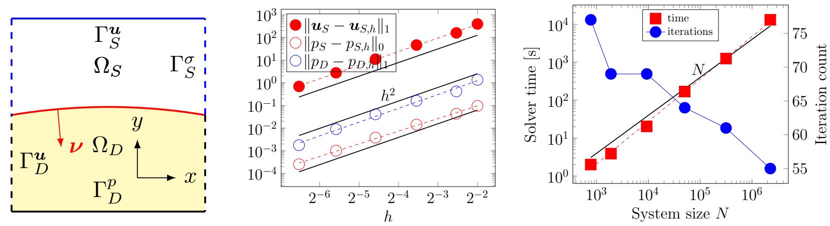

Fig. 5 (Left) Computation domain is obtained by extrusion of the pictured geometry. The interface Γ, being part of a circle arc, is curved. No-slip and traction conditions are prescribed on $\Gamma_S^{\boldsymbol{u}}$ and Γ_S^{σ} respectively. Darcy pressure is prescribed on Γ_D^{p}. (Center) Error convergence study performed using the $3d$ setup. With $\mathbb{P}_2$-$\mathbb{P}_1$-$\mathbb{P}_2$ elements, optimal quadratic rates are observed in all the variables. (Right) Solver time (including preconditioner setup and FGMRes runtime) scales linearly with the problem size.

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