Imperial College London

14 July 2023

Numerical analysis of finite element methods for topology optimization problems

IMA Leslie Fox Prize 2023

Ioannis Papadopoulos

Topology optimization

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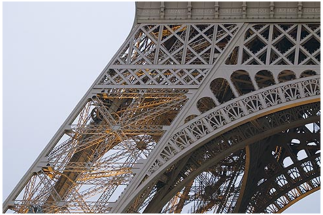

(a) TO of compliance.
https://tinyurl.com/523ep9av

(b) TO of compliance.
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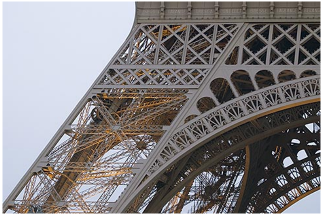
Topology optimization



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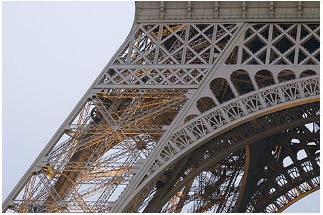

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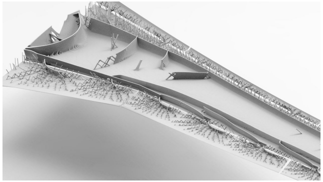
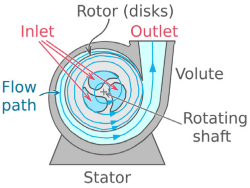
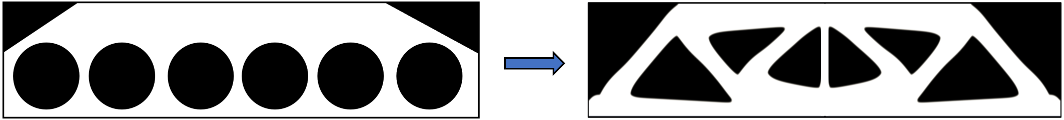


(d) Aage et al., *Nature* (2017).

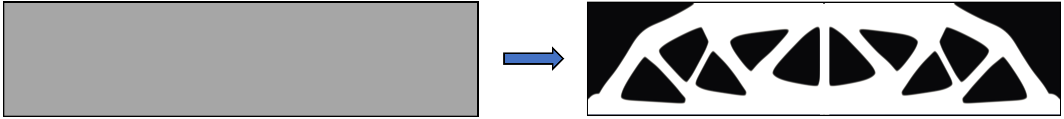


(e) Alonso et al., *CAMWA* (2019).

Shape vs. topology optimization



(a) Shape optimization



(b) Topology optimization

Models & optimization strategies

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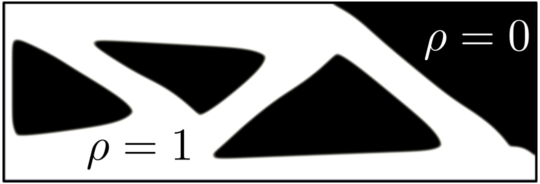
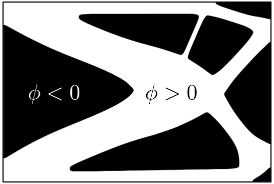
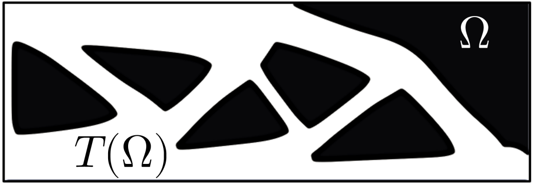
The model for representing the topology of the minimizer:



(a) Density.



(b) Level-set.



(c) Admissible domain maps.

The main textbook describing the density approach (Bendsoe, Sigmund, 2003) has $\sim 10,000$ citations. Over 20 professional software packages, consulting firms etc.

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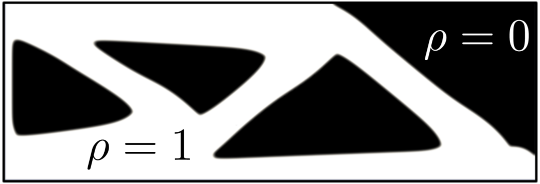

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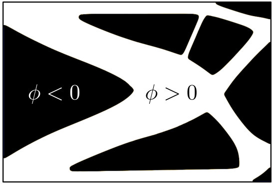

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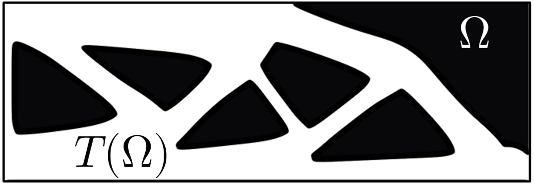

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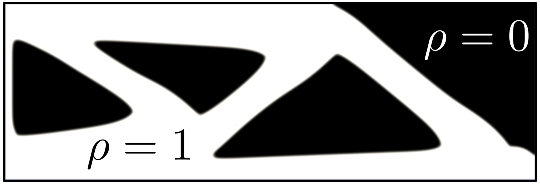

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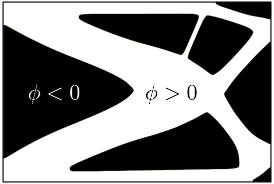

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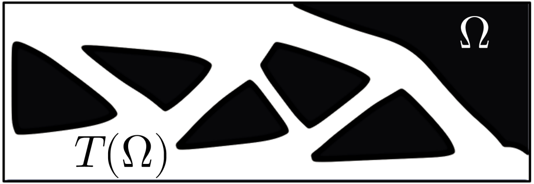

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Numerical difficulties

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Models for topology optimization problems tend to:

- involve PDEs $\implies$ require a discretization, e.g. the finite element method (FEM).
- be nonconvex $\implies$ may support multiple local minima.

Open questions

- What is the best model?
- How do we interpret regions that are neither completely void or continuum?
- Do discretizations of the models actually converge to the minimizers of the original problem?
- Are the discretizations well behaved?
- Can we prove error bounds?
- Is there a general framework for proving convergence of FEM to all (density-based) topology optimization problems?

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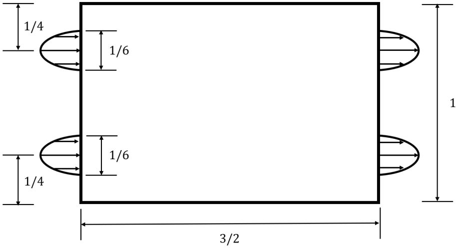
The Borrvall–Petersson problem



Double-pipe problem

A fluid topology optimization problem

- Stokes flow.
- Wish to minimize the power dissipation of the flow;
- Catch! The channels can occupy up to 1/3 area.
- Requires solving a nonconvex optimization problem with PDE, box, and volume constraints.

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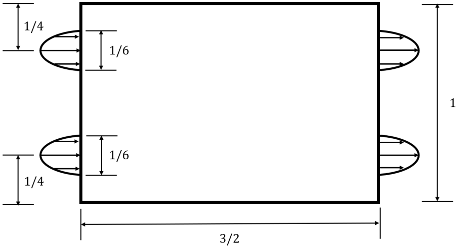

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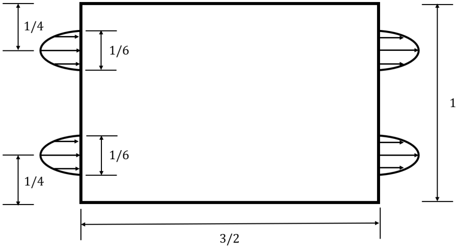

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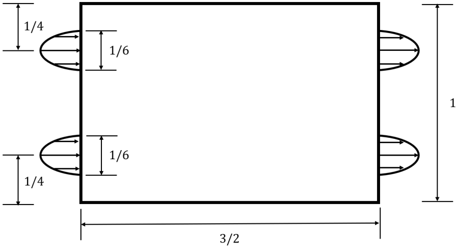

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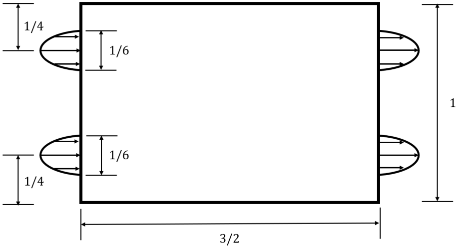

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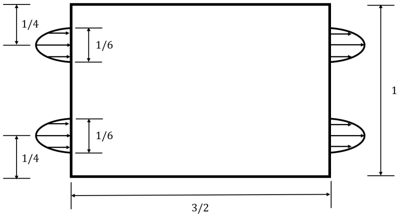
Double-pipe solutions



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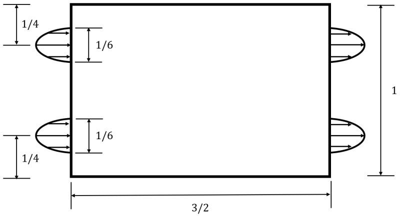

(a) Straight channels

Double-pipe solutions

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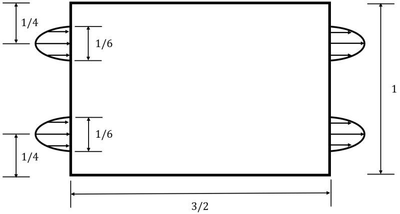


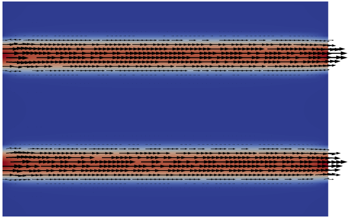
(a) Straight channels

(b) Double-ended wrench

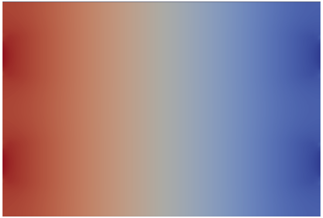
What functions are we solving for?

Given that the fluid can only occupy 1/3 of the total domain, we are solving for:

Material distribution
$\rho : \Omega \to [0, 1]$



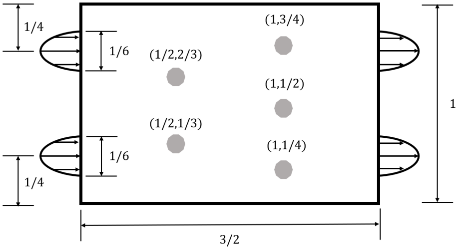
Velocity
$u : \Omega \to \mathbb{R}^2$



Pressure
$p : \Omega \to \mathbb{R}$

Red is where $\rho = 1$ and blue is where $\rho = 0$.

A fluid topology optimization problem

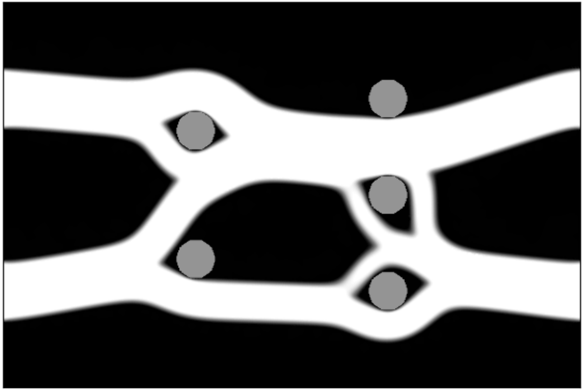


Five-holes double-pipe setup.

Fluid topology optimization

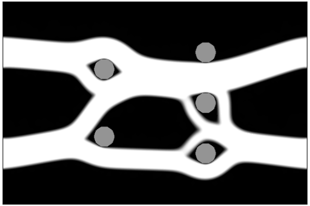
- Navier–Stokes flow.
- Wish to minimize the power dissipation of the flow;
- Catch! The channels can occupy up to $1/3$ area.

A fluid topology optimization problem



$$J = 60.09$$

A fluid topology optimization problem



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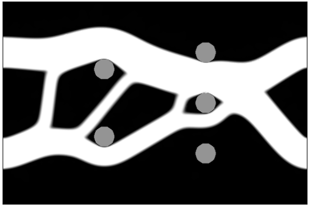
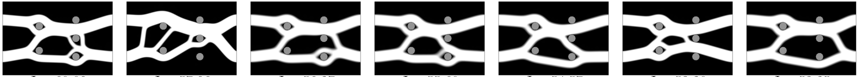


$J = 57.96$

A fluid topology optimization problem



$J = 60.09$ $J = 57.96$ $J = 56.27$ $J = 55.60$ $J = 54.57$ $J = 53.20$ $J = 53.25$

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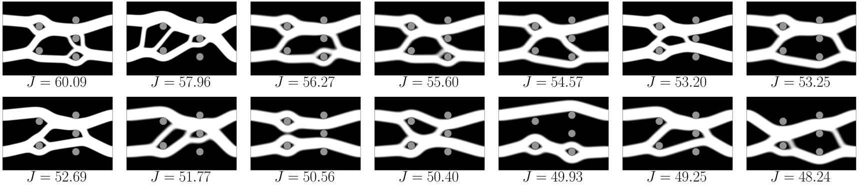

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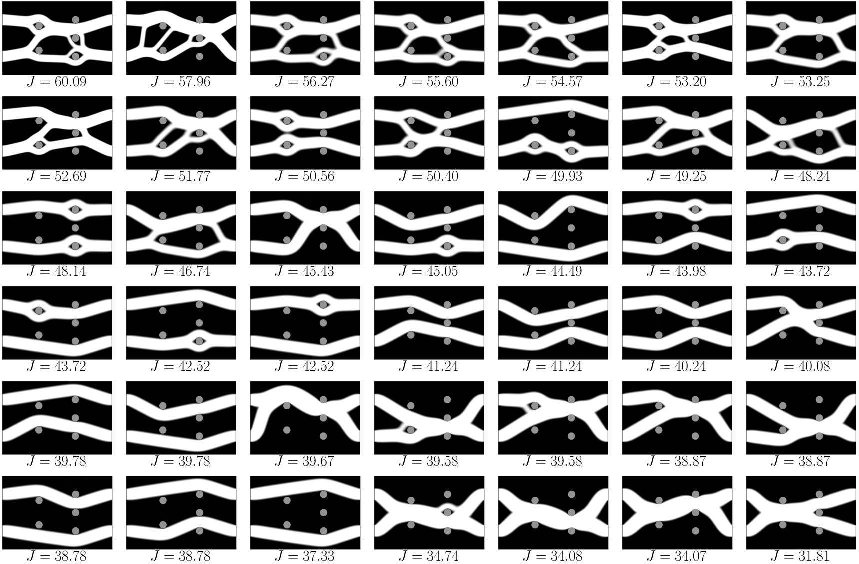
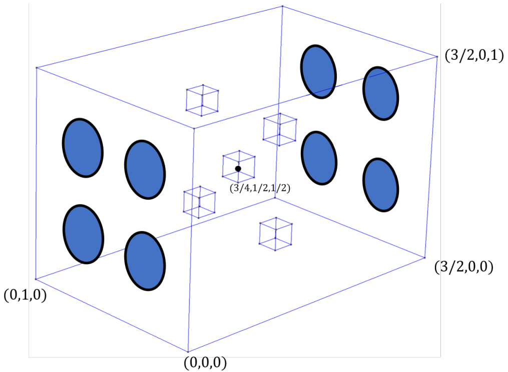


3D five-holes quadruple-pipe

3D Borrvall–Petersson problem

- Stokes flow;
- Minimize the power dissipation;
- Channels can occupy up to $1/5$ of the volume of the box.



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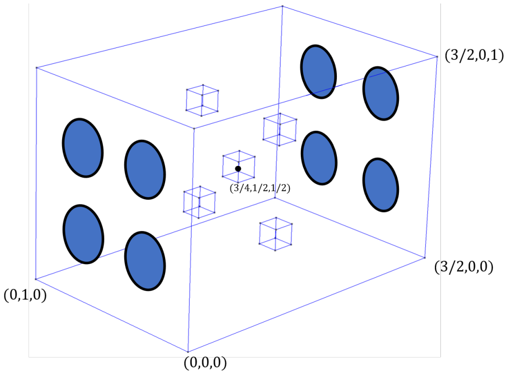

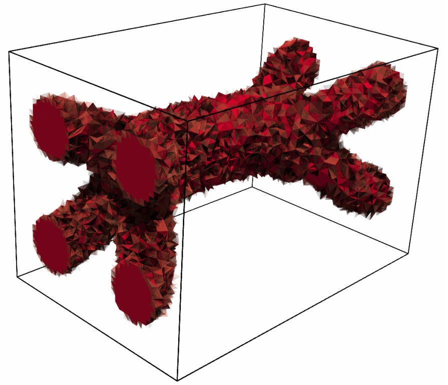

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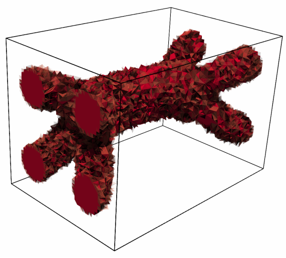

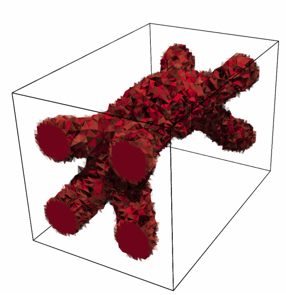

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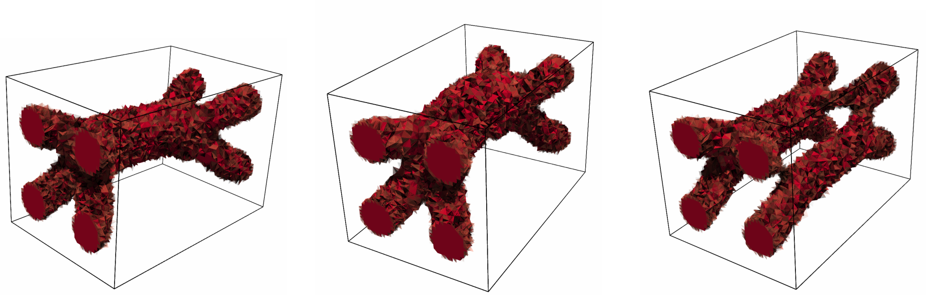

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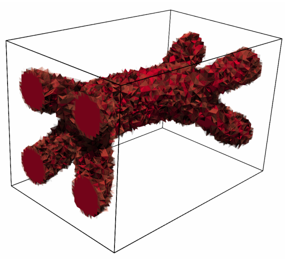

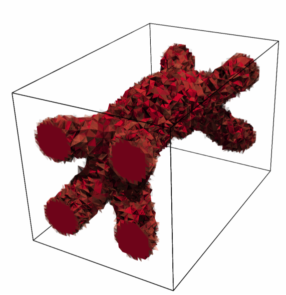

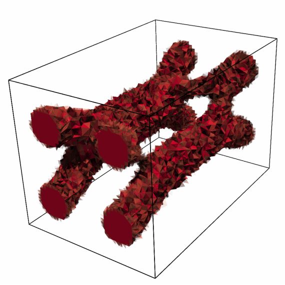

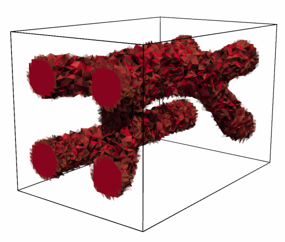

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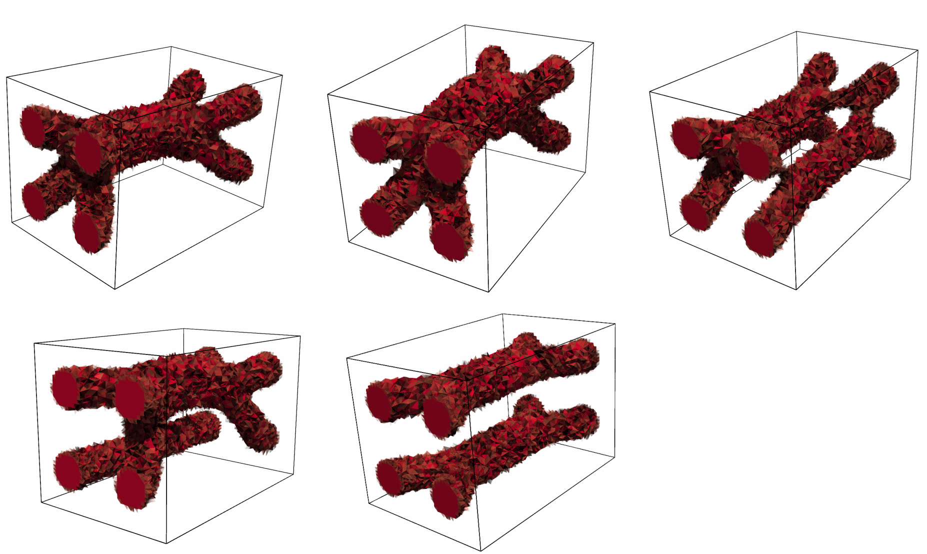

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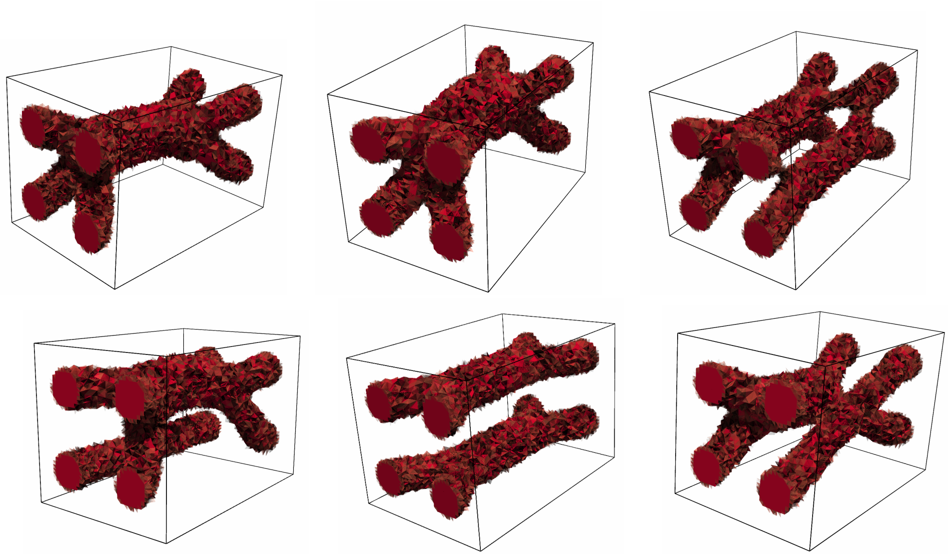

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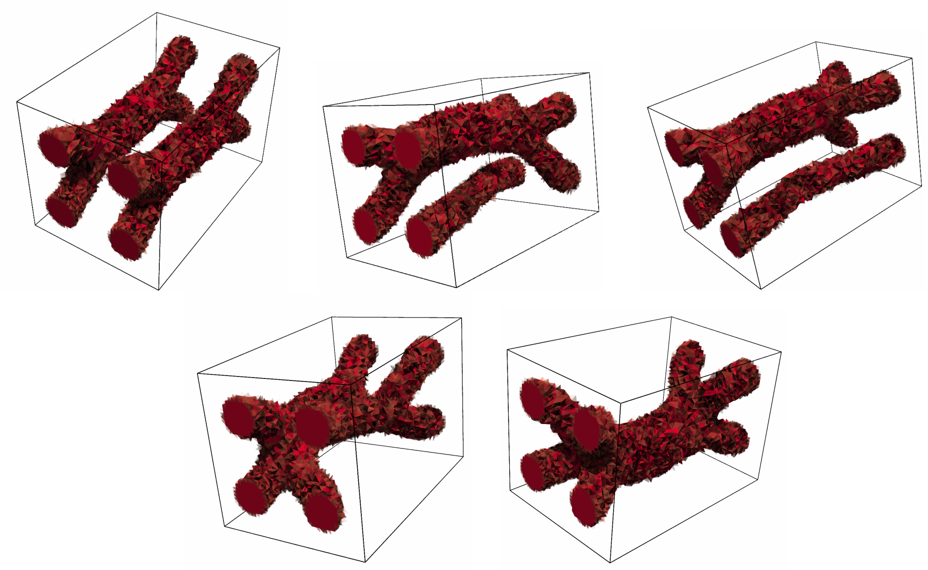
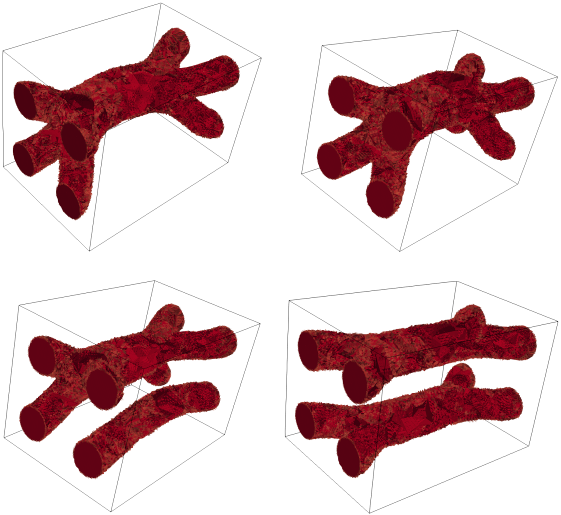


Refinement of 3D five-holes quadruple-pipe



15,953,537 degrees of freedom.

Choice of discretization

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Observations

- Many solutions to approximate.
- Mesh adaptivity strategies.
- Millions of degrees of freedom.
- Parameters may vary between 0 and 10^{10}.

Consequences

We require preconditioners for the solves e.g. effective multigrid cycles & small errors in the velocity, material distribution, and pressure discretizations.

Our proposal

Use a discontinuous Galerkin (DG) mixed finite element where $\|\mathrm{div}(u_h)\|_{L^2(\Omega)} = 0^\dagger$.

Question

Does the discretization converge to the (multiple) infinite-dimensional* minimizers?

† $_h$ denotes the mesh size in the FEM discretization.

* An "infinite-dimensional" minimizer is a minimizer of the original problem before discretization.

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- Many solutions to approximate.
- Millions of degrees of freedom.
- Mesh adaptivity strategies.
- Parameters may vary between 0 and 10^{10}.

Consequences

We require preconditioners for the solves e.g. effective multigrid cycles & small errors in the velocity, material distribution, and pressure discretizations.

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Use a discontinuous Galerkin (DG) mixed finite element where $\|\mathrm{div}(u_h)\|_{L^2(\Omega)} = 0^{\dagger}$.

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Does the discretization converge to the (multiple) infinite-dimensional* minimizers?

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Topology optimization of fluid flow

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Generalized Stokes equations

$$\alpha(\rho)u - \nu\Delta u + \nabla p = f, \qquad \text{(Momentum equation)} \tag{1}$$

$$\operatorname{div}(u) = 0, \qquad \text{(Incompressibility)} \tag{2}$$

$$u|_{\partial\Omega} = g. \qquad \text{(Boundary conditions)} \tag{3}$$

$\alpha(\cdot)$ is an inverse permeability term.

$$\rho = 1, \text{ Momentum equation} \approx \quad -\nu\Delta u + \nabla p = f \implies \text{Stokes},$$

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Find the velocity, u, and the material distribution, ρ, that minimize

$$J(u,\rho) := \frac{1}{2}\int_\Omega \left(\alpha(\rho)|u|^2 + \nu|\nabla u|^2 - 2f\cdot u\right) \mathrm{d}x,$$

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α has the following properties:

1. $\alpha : [0, 1] \to [\underline{\alpha}, \overline{\alpha}]$ with $0 \le \underline{\alpha}$ and $\overline{\alpha} < \infty$;
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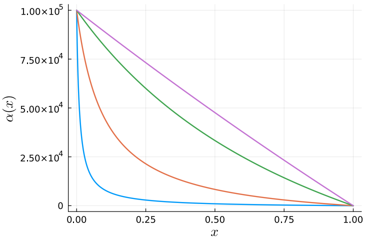

generating an operator also denoted $\alpha : C_\gamma \to L^\infty(\Omega; [\underline{\alpha}, \overline{\alpha}])$.

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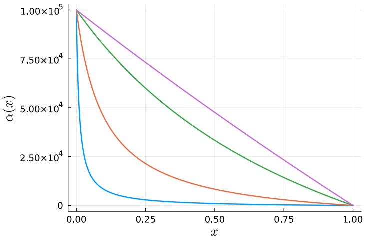

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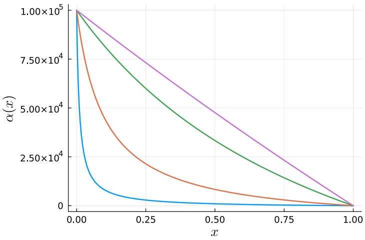

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First-order optimality conditions

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Types of convergence

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Strong convergence

$z_n \to z$ strongly in $L^q(\Omega)$ if $\lim_{n\to\infty} \|z_n - z\|_{L^q(\Omega)} = 0$.

Weak convergence

$z_n \rightharpoonup z$ weakly in $L^q(\Omega)$, if for all $v \in L^{q'}(\Omega)$, $1/q' + 1/q = 1$,

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Weak-* convergence in $L^\infty(\Omega)$

If $z_n \in L^\infty(\Omega)$, then $z_n \overset{*}{\rightharpoonup} z$ weakly-* in $L^\infty(\Omega)$, if for all $v \in L^1(\Omega)$, $\int_\Omega z_n v \, \mathrm{d}x \to \int_\Omega z v \, \mathrm{d}x$.

Weak convergence $\not\Rightarrow$ strong convergence

$\sin(nx) \rightharpoonup 0$ weakly in $L^2([0, 2\pi])$, but $\|\sin(nx) - 0\|_{L^2([0,2\pi])} = \pi$ for all $n \in \mathbb{Z}_+$.

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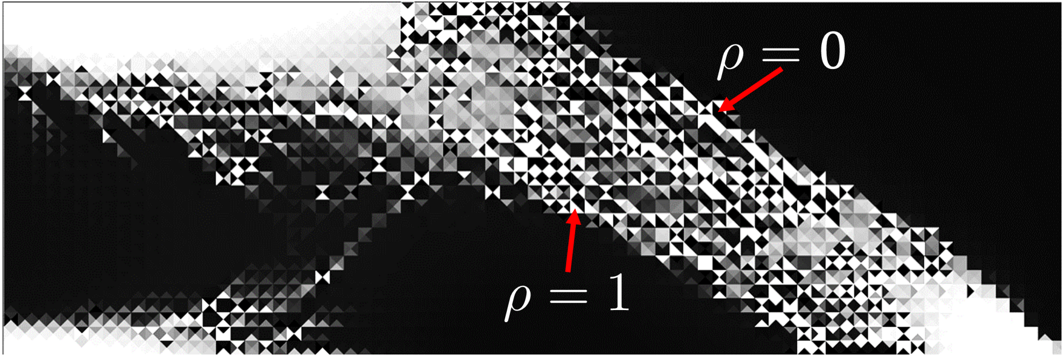
Poor behaviour of weak-* convergence



Formation of checkerboard patterns.

Motivation for DG methods

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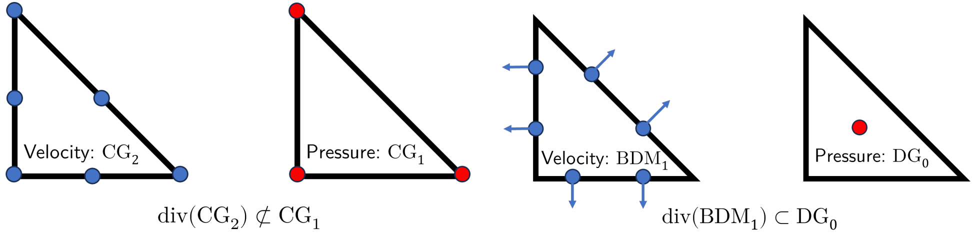
Throughout $\rho_h \in C_\gamma$ and $p_h \in L^2(\Omega)$.

Conforming $\implies u_h \in H^1(\Omega)^d$, Divergence-free DG $\implies u_h \notin H^1(\Omega)^d$.



(a) Taylor–Hood pair (b) Brezzi–Douglas–Marini pair

1. Both pairs satisfy an inf-sup condition;
2. The Taylor–Hood pair is continuous across cells and $\mathrm{CG}_2 \subset H^1(\Omega)^2$;
3. The BDM pair only enforces continuity in the normal direction across cells, $\mathrm{BDM}_1 \not\subset H^1(\Omega)^2$;
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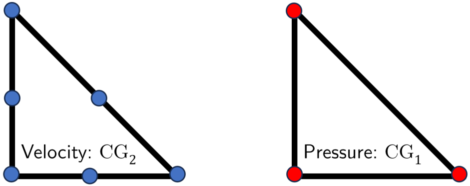
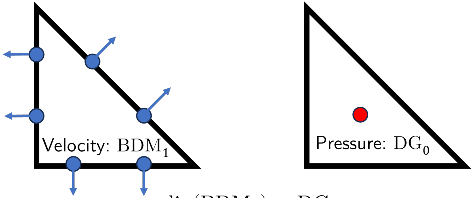


$\mathrm{div}(\mathrm{CG}_2) \not\subset \mathrm{CG}_1$

(a) Taylor–Hood pair



$\mathrm{div}(\mathrm{BDM}_1) \subset \mathrm{DG}_0$

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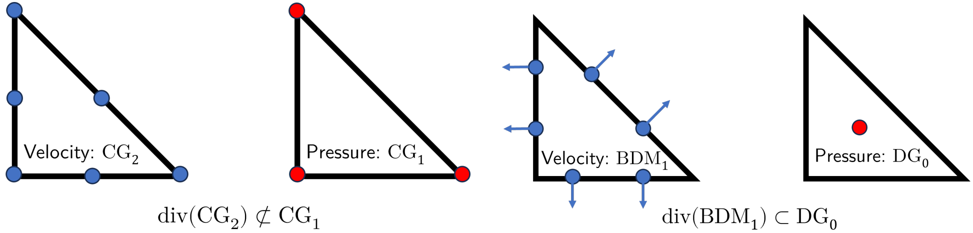

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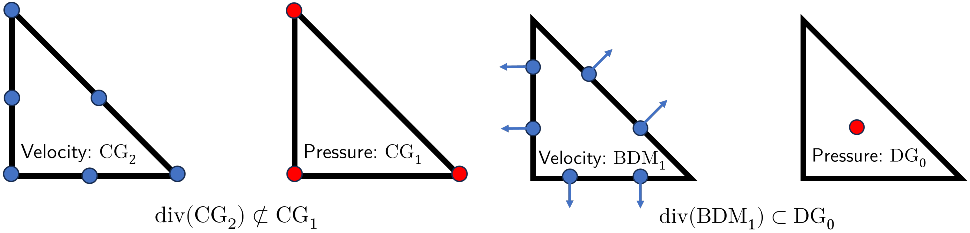

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Finite element convergence

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$$J_h(u_h, \rho_h) := \frac{1}{2}\int_\Omega \left(\alpha(\rho_h)|u_h|^2 - 2f \cdot u_h\right) \mathrm{d}x$$

$$\frac{\nu}{2}\int_\Omega |\nabla u_h|^2 \,\mathrm{d}x \approx \begin{cases} +\frac{\nu}{2}\sum_{K\in\mathcal{T}_h}\int_K |\nabla u_h|^2 \mathrm{d}x \\ -\nu \sum_{F\in\mathcal{F}_h^i}\int_F \{\!\{\nabla u_h\}\!\}_F : [\![u_h]\!]_F \,\mathrm{d}s \\ -\nu \sum_{F\in\mathcal{F}_h^\partial}\int_F \{\!\{\nabla u_h\}\!\}_F : [\![u_h - g_h]\!]_F \,\mathrm{d}s \end{cases}$$

$$\text{Penalty for continuity} \begin{cases} +\frac{\nu}{2}\sum_{F\in\mathcal{F}_h^i}\sigma h_F^{-1}\int_F |[\![u_h]\!]_F|^2 \mathrm{d}s \\ +\frac{\nu}{2}\sum_{F\in\mathcal{F}_h^\partial}\sigma h_F^{-1}\int_F |[\![u_h - g_h]\!]_F|^2 \mathrm{d}s \end{cases}$$

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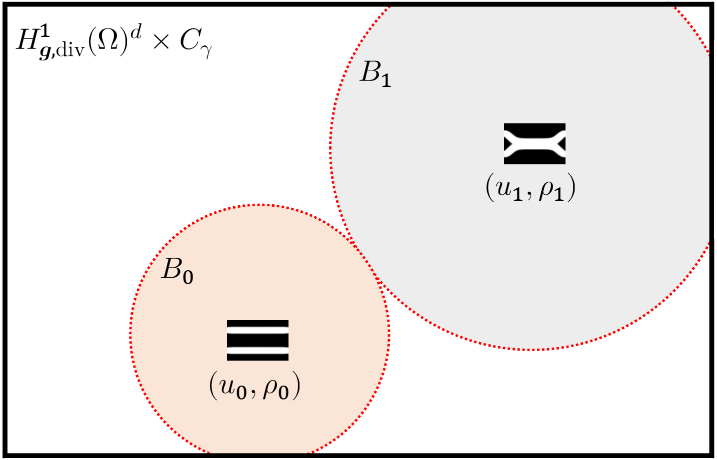
Outline of FEM convergence proof

Key idea: fix an isolated local minimizer (u, ρ).



Outline of FEM convergence proof

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Consider the modified finite-dimensional optimization problem:

$$\text{Find } (u_h^*, \rho_h^*) \in B \cap (V_h \times C_{\gamma,h}) \text{ that minimizes } J_h(v_h, \eta_h). \tag{*}$$

$$u_h \notin H^1(\Omega)^d, \;\; V_h \not\subset H^1_{g,\mathrm{div}}(\Omega)^d \;\; \text{and} \;\; C_{\gamma,h} \subset C_\gamma.$$

(u_h^*, ρ_h^*) is not computable in practice.

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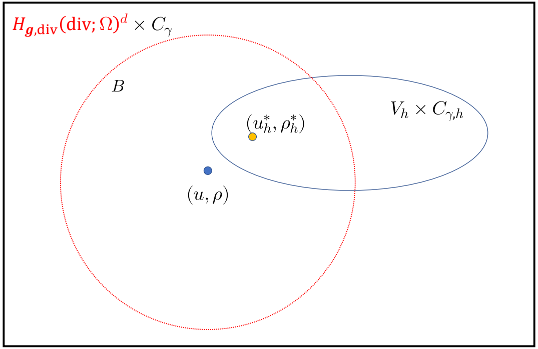

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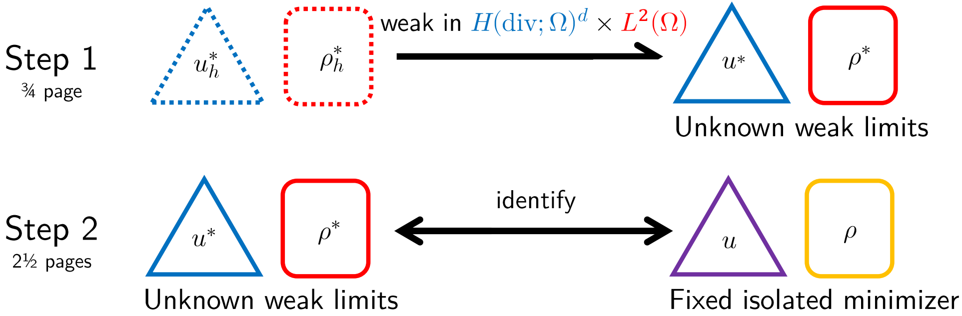

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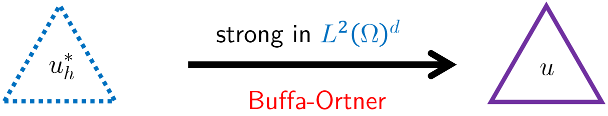
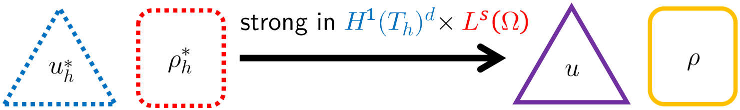
Step 3
½ page



Step 4
5 pages



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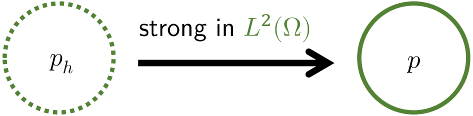
Step 5
¾ page

Subsequence

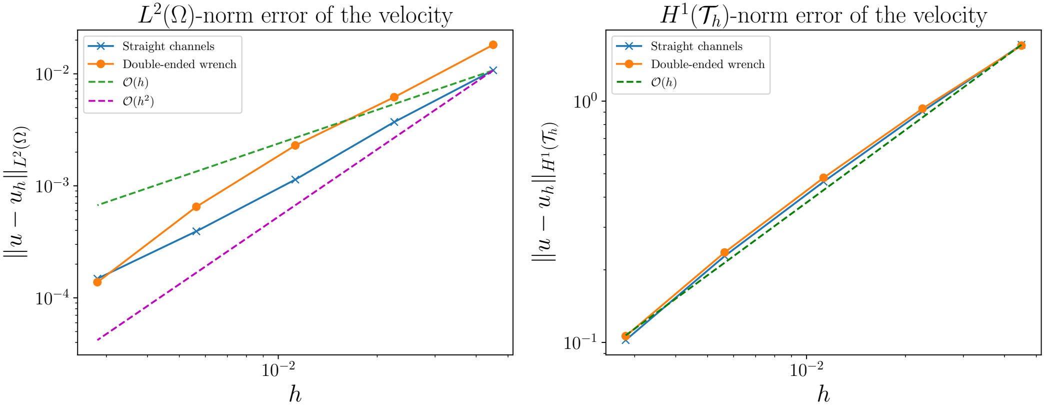
No dependence on B. One may solve the discretized FOCs for (u_h, ρ_h, p_h)

Step 6
1 page



QED.

Numerical examples



Convergence of the double-pipe problem on a sequence of uniformly refined meshes with a $\mathrm{DG}_0 \times \mathrm{BDM}_1 \times \mathrm{DG}_0$ discretization for (ρ_h, u_h, p_h).

Numerical examples

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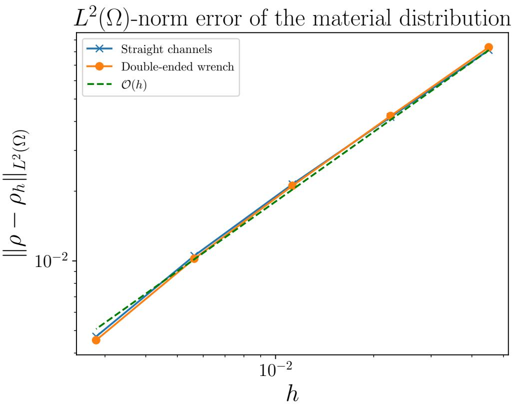

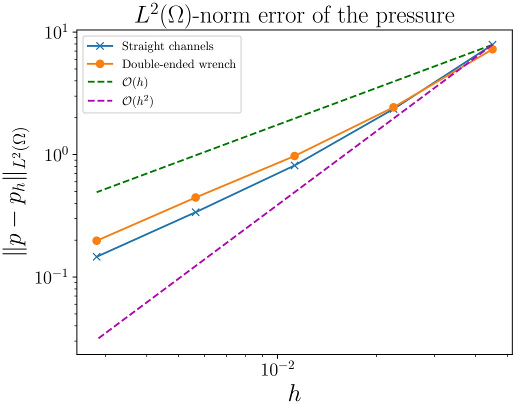

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Numerical examples

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	Straight channels		Double-ended wrench	
h	BDM	Taylor–Hood	BDM	Taylor–Hood
4.51×10^{-2}	1.00×10^{-8}	2.49×10^{-1}	2.69×10^{-6}	3.25×10^{-1}
2.25×10^{-2}	6.35×10^{-9}	1.09×10^{-1}	2.75×10^{-8}	1.35×10^{-1}
1.13×10^{-2}	1.59×10^{-7}	3.95×10^{-2}	2.62×10^{-8}	4.66×10^{-2}
5.63×10^{-3}	4.19×10^{-8}	1.19×10^{-2}	1.48×10^{-7}	1.36×10^{-2}
2.82×10^{-3}	4.97×10^{-7}	3.17×10^{-3}	2.98×10^{-7}	3.58×10^{-3}

Table 1: Reported values for $\|\mathrm{div}(u_h)\|_{L^2(\Omega)}$ in a BDM and Taylor–Hood discretization for the double-pipe problem as measured on five meshes in a uniformly refined mesh hierarchy.

Future work

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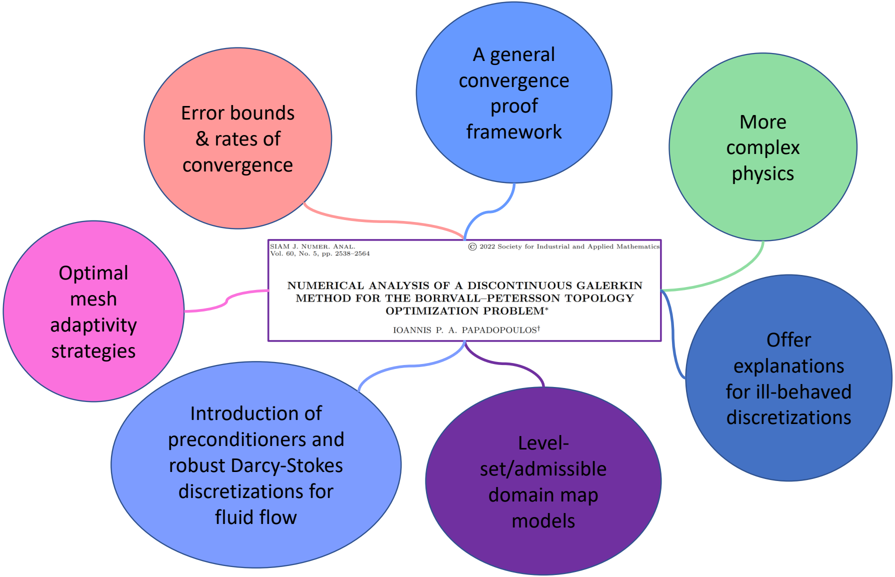

Conclusions

Imperial College London

- Solutions of 3D Borrvall–Petersson problems are useful $\implies$ requires preconditioners and low errors $\implies$ use a divergence-free DG finite element for the velocity-pressure pair.
- This talk outlines the proof of strong convergence for the divergence-free DG discretization.
- Forms the basis for proving useful results including optimal mesh adaptivity strategies and well-behaved discretizations.

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I. P, SIAM Journal on Numerical Analysis, 2022. https://doi.org/10.1137/21M1438943.

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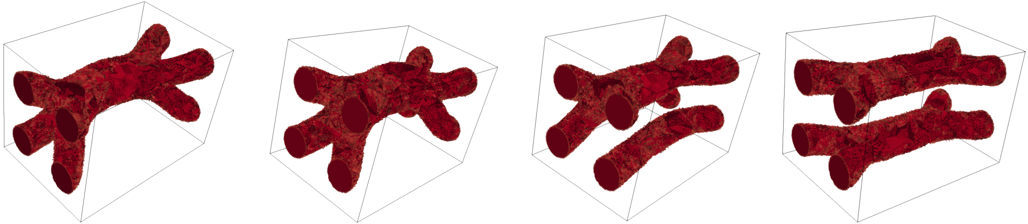
Thank you for listening!

✉ ioannis.papadopoulos13@imperial.ac.uk



A solver for computing multiple solutions

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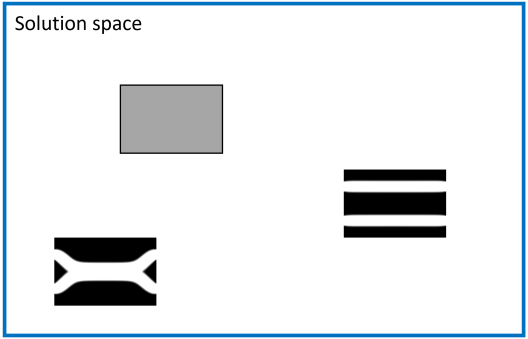
Deflated barrier method

Continuation scheme + primal-dual active set strategy + deflation



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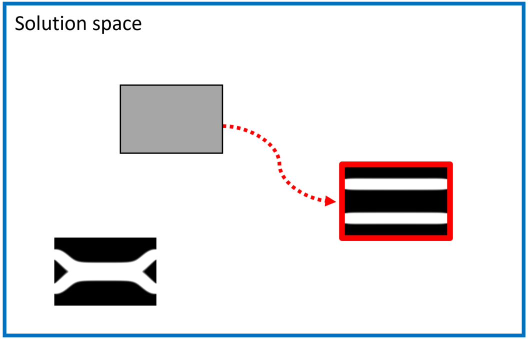

Step I: optimize from initial guess

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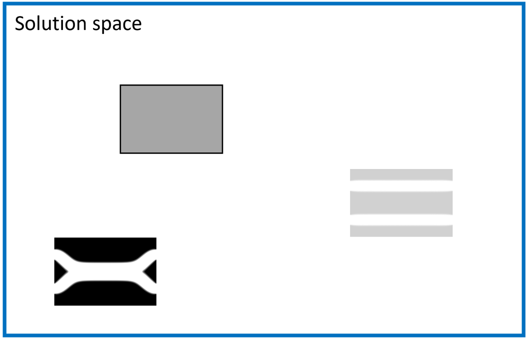

Step II: deflate solution found

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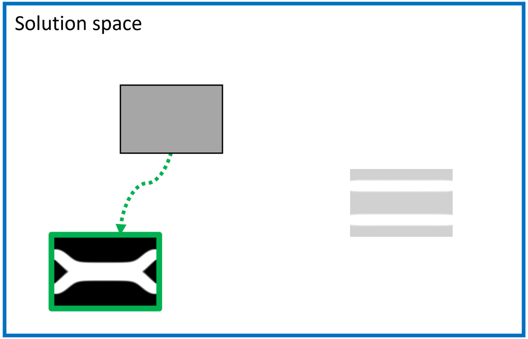

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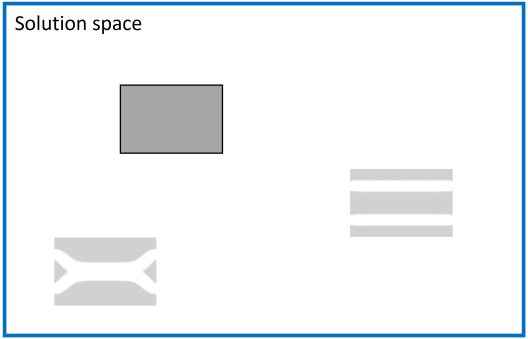

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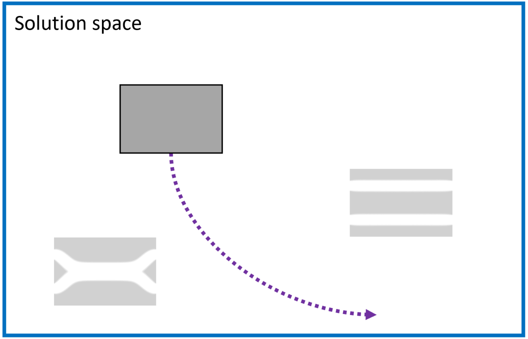

Step III: termination on nonconvergence

Construction of deflated problems

A nonlinear transformation of first-order optimality conditions

$$\mathcal{F}(z) = 0 \to \mathcal{G}(z) := \mathcal{M}(z; r)\mathcal{F}(z) = 0.$$

A deflation operator

We say that $\mathcal{M}(z; r)$ is a deflation operator if for any sequence $z \to r$

$$\liminf_{z \to r} \|\mathcal{G}(z)\| = \liminf_{z \to r} \|\mathcal{M}(z; r)\mathcal{F}(z)\| > 0.$$

Theorem

This is a deflation operator for $p \geq 1$:

$$\mathcal{M}(z; r) = \left(\frac{1}{\|z - r\|^p} + 1\right).$$

Construction of deflated problems

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