Computing multiple solutions of topology optimization problems

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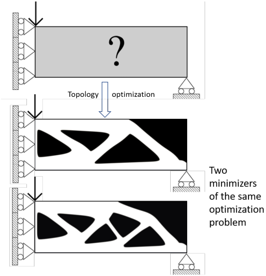
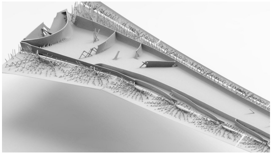
Topology optimization

Models for topology optimization problems tend to:

- involve PDEs $\implies$ require a discretization;
- be nonconvex $\implies$ may support multiple local minima.





Aage, Andreassen, Lazarov, Sigmund, *Nature* (2017)

In this talk we will solely consider density-based models & FEM discretizations.

Choice of optimization strategy

Observations

- Potentially many (local) minimizers.
- Millions of degrees of freedom.

Consequences

- Require algorithms that converge quickly.
- Compute multiple minimizers in a systematic manner.
- Require preconditioners for the solves e.g. effective multigrid cycles.

Our proposal

The deflated barrier method.

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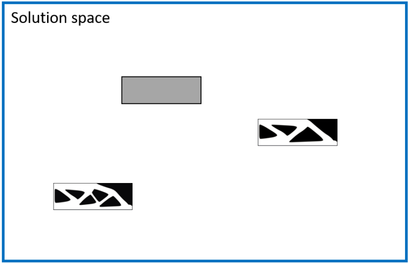
Barrier-like terms + primal-dual active set strategy + deflation



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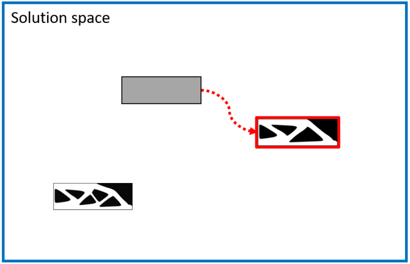
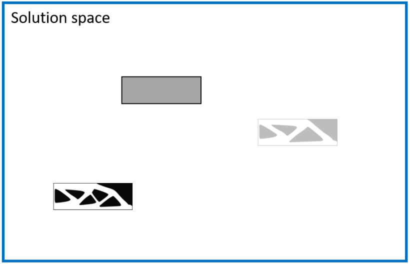


Step I: optimize from initial guess

The deflated barrier method

Deflated barrier method

Barrier-like terms + primal-dual active set strategy + deflation



Step II: deflate solution found

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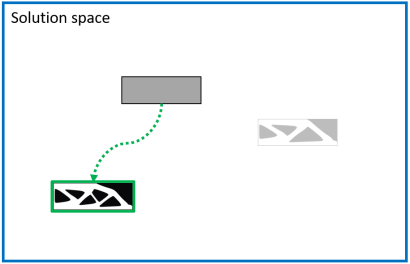

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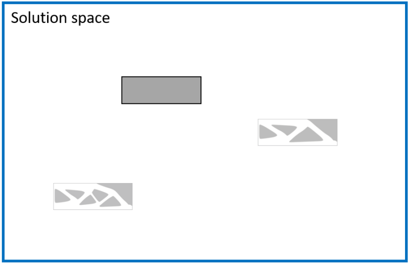

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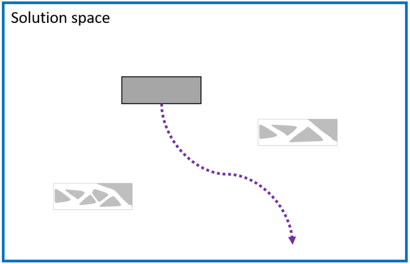

Step III: termination on nonconvergence

Construction of deflated problems

A nonlinear transformation of a nonlinear system

$$F(x) = 0 \;\text{ has the solutions } x_1, \ldots, x_n.$$

Via, e.g. Newton's method, we discover x_1.

$$G(x) := \mathcal{M}(x; x_1)F(x) = 0 \;\text{ has the solutions } x_2, \ldots, x_n, \text{ but not } x_1!$$

A deflation operator

We say that $\mathcal{M}(x; x_1)$ is a deflation operator for F if (1) it is invertible $\forall x \neq x_1$ in a neighborhood of x_1 and (2) for any sequence $x \to x_1$

$$\liminf_{x \to x_1} \|G(x)\| = \liminf_{x \to x_1} \|\mathcal{M}(x; x_1)F(x)\| > 0.$$

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Construction of deflated problems

Theorem

Suppose F is *semismooth* at x_1 and its Newton derivative is invertible and bounded. Then the following is a deflation operator for F:

$$\mathcal{M}(x; x_1) = \left(\frac{1}{\|x - x_1\|^p} + 1 \right), \quad \text{for any } p \geq 1.$$

After discretization, deflation is *very* easy to implement!

Step 1

Compute the *undeflated* Newton update $\delta x_F = -[F'(x)]^{-1} F(x)$.

Step 2

Let $m = m(x) = \mathcal{M}(x; x_1)$. Then the deflated Newton update satisfies

$$\delta x_G = \tau(x, \delta x_F)\delta x_F \text{ where } \tau(x, \delta x) := \left(1 + \frac{m^{-1}\langle m', \delta x\rangle}{1 - m^{-1}\langle m', \delta x\rangle} \right).$$

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Leibniz Association

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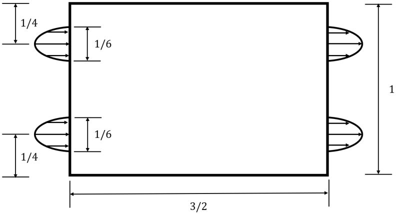

Double-pipe problem

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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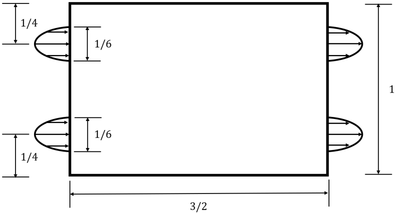

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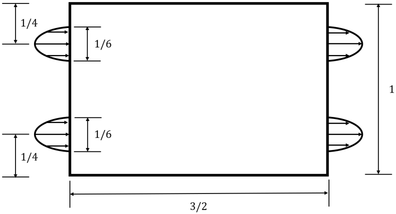

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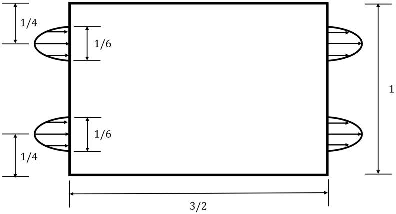

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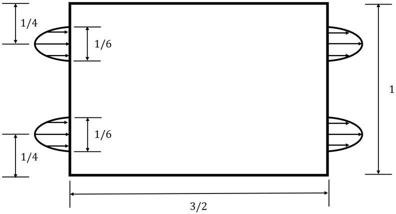

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Borrvall & Petersson

T. Borrvall and J. Petersson derived the "generalized Stokes equations":

$$\alpha(\rho)u - \nu\Delta u + \nabla p = f, \quad (1)$$

$$\mathrm{div}(u) = 0, \quad (2)$$

$$u|_{\partial\Omega} = g. \quad (3)$$

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

Common choice: $\alpha(\rho) = \bar{\alpha}\left(1 - \frac{\rho(q+1)}{\rho+q}\right), \bar{\alpha} \gg 0, q > 0.$

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

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Find velocity $u \in H^1(\Omega)^2$ and density $\rho \in L^\infty(\Omega)$ that minimize

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

subject to $\mathrm{div}(u) = 0$, $u|_{\partial\Omega} = g$, $0 \le \rho \le 1$, and $\int_\Omega \rho \, \mathrm{d}x \le \frac{1}{3}|\Omega|$.

FEM discretization: I. P., E. Süli, *J. Comput. Appl. Math* (2022)

Consider an isolated minimizer (u, p, ρ) of the Borrvall–Petersson problem.

- (u, p) is discretized with a conforming inf-sup stable FEM discretization.
- Density ρ is discretized with an L^2-conforming discretization.

Then there exists a sequence of discretized solutions such that
$(u_h, p_h, \rho_h) \to (u, p, \rho)$ strongly in $H^1(\Omega)^d \times L^2(\Omega) \times L^s(\Omega)$ for $1 \le s < \infty$.

E.g. use Taylor–Hood (P2-P1) for (u, p) and continuous P1 for ρ.

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$(u_h, p_h, \rho_h) \to (u, p, \rho)$ strongly in $H^1(\Omega)^d \times L^2(\Omega) \times L^s(\Omega)$ for $1 \leq s < \infty$.

E.g. use Taylor–Hood (P2-P1) for (u, p) and continuous P1 for ρ.

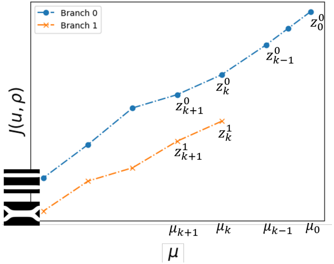
Leibniz Association

The deflated barrier method
Overview

Deflated barrier method

For $\mu = \mu_0$ ($\mu \to 0$), solve $\nabla L_\mu(u, \rho, p, \lambda)$ "=" 0 with a primal-dual active set strategy where

$$L_\mu(u,\rho,p,\lambda) = J(u,\rho) - \int_\Omega p\,\mathrm{div}(u) + \lambda(1/3 - \rho)\,\mathrm{d}x - \mu \int_\Omega \log((\rho+\epsilon)(1+\epsilon-\rho))\,\mathrm{d}x.$$



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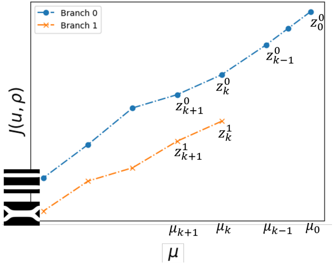

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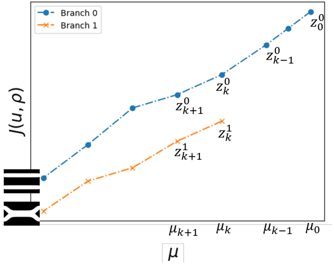

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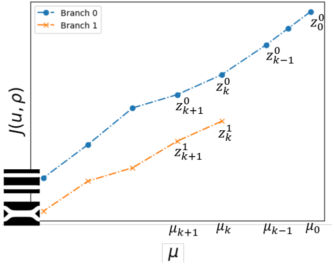
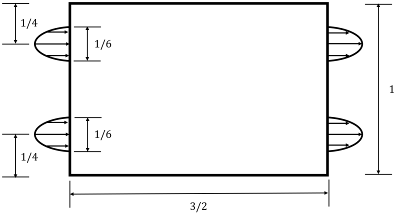


The Borrvall–Petersson problem



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.

Double-pipe solutions

(a) Straight channels

Double-pipe solutions

(a) Straight channels

(b) Double-ended wrench

Double-pipe solutions

(a) Straight channels

(b) Double-ended wrench

(c) Neumann (i)

Double-pipe solutions

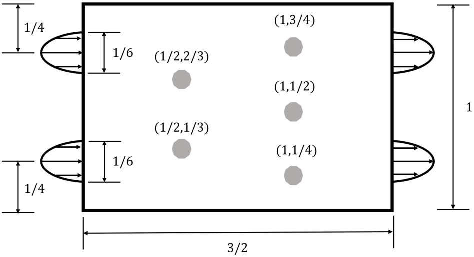
(a) Straight channels

(b) Double-ended wrench

(c) Neumann (i)

(d) Neumann (ii)

A fluid topology optimization problem

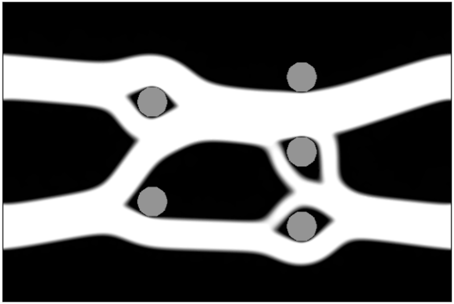


Five-holes double-pipe setup.

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
Five-holes double-pipe

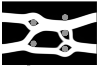


$$J = 60.09$$

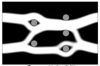
A fluid topology optimization problem
Five-holes double-pipe

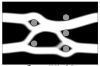
$J = 60.09$ $J = 57.96$

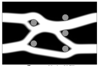
A fluid topology optimization problem
Five-holes double-pipe

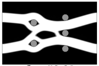

$J = 60.09$

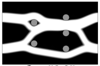

$J = 57.96$


$J = 56.27$

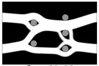

$J = 55.60$


$J = 54.57$


$J = 53.20$


$J = 53.25$

A fluid topology optimization problem
Five-holes double-pipe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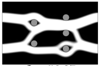
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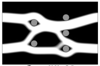
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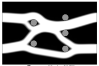
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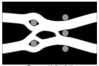
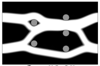

$J = 53.20$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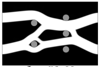
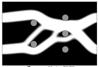
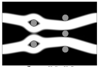
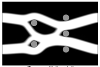
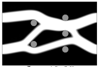

$J = 52.69$


$J = 51.77$


$J = 50.56$


$J = 50.40$


$J = 49.93$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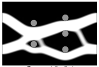
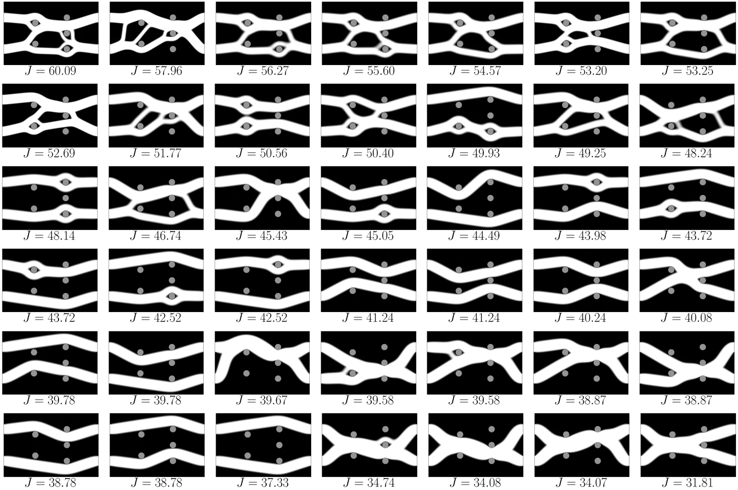
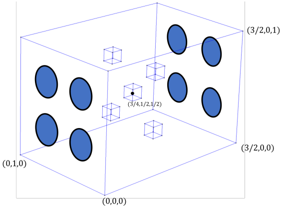

$J = 48.24$

A fluid topology optimization problem
Five-holes double-pipe



Examples
3D quadruple-pipe

- 3D discretization on a $40 \times 40 \times 40$ block $\sim$ 3,000,000 dofs.
- (Stokes) Nevertheless still numerically tractable via preconditioning techniques.



FEM discretization: I. P., *SINUM* (2022)

- (u, p) is discretized with a *non-conforming div-free inf-sup stable discretization* and an interior penalty is added.
- Density ρ is discretized with an L^2-conforming discretization.

Then there exists a sequence of discretized solutions such that

$$(u_h, p_h, \rho_h) \to (u, p, \rho) \text{ strongly in } H^1(\mathcal{T}_h)^d \times L^2(\Omega) \times L^s(\Omega) \text{ for } 1 \leq s < \infty.$$

E.g. Brezzi–Douglas–Marini with IP for (u, p) and piecewise constant for ρ.

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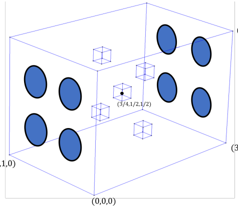

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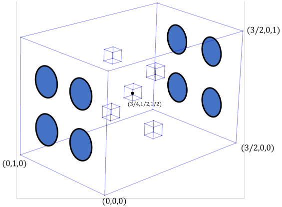

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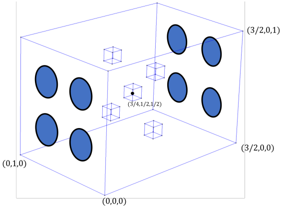

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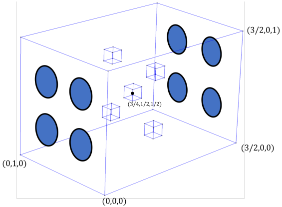

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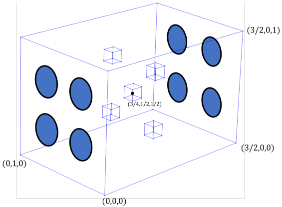

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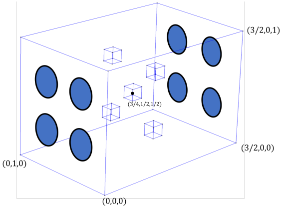

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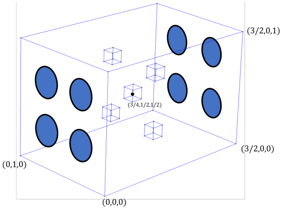

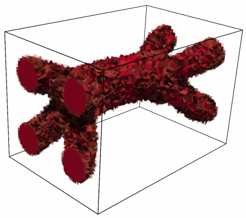

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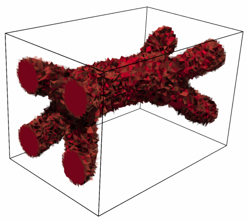
3D five-holes quadruple-pipe



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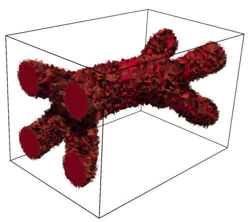

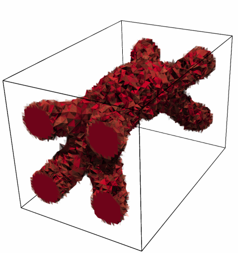

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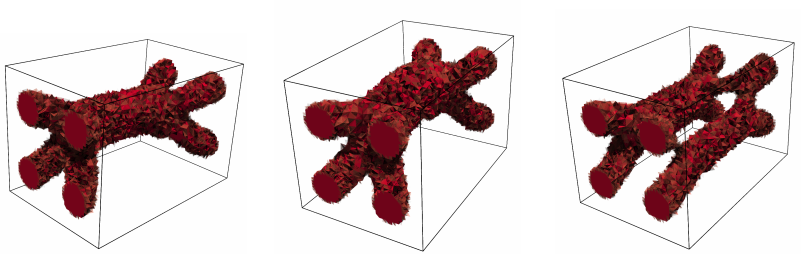

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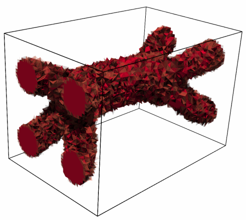

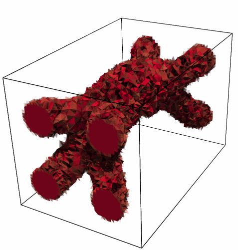

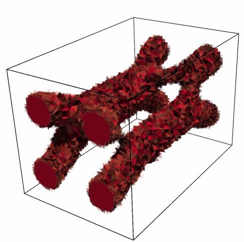

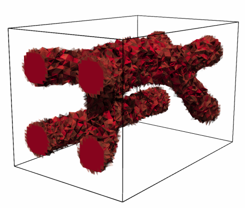

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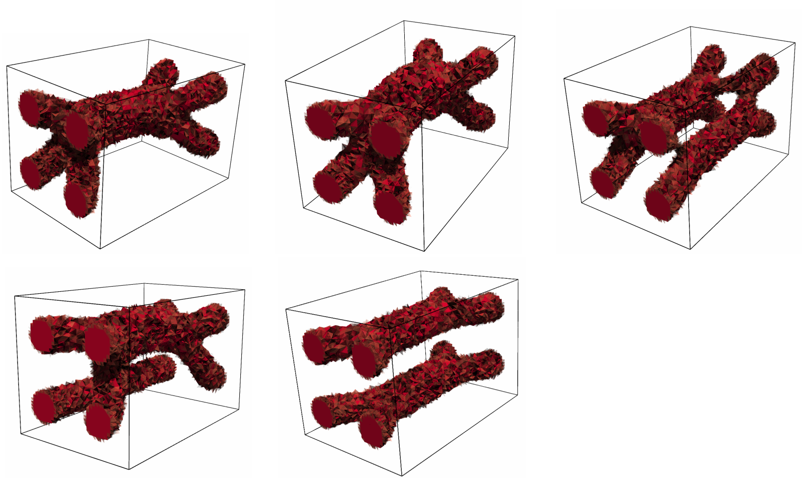

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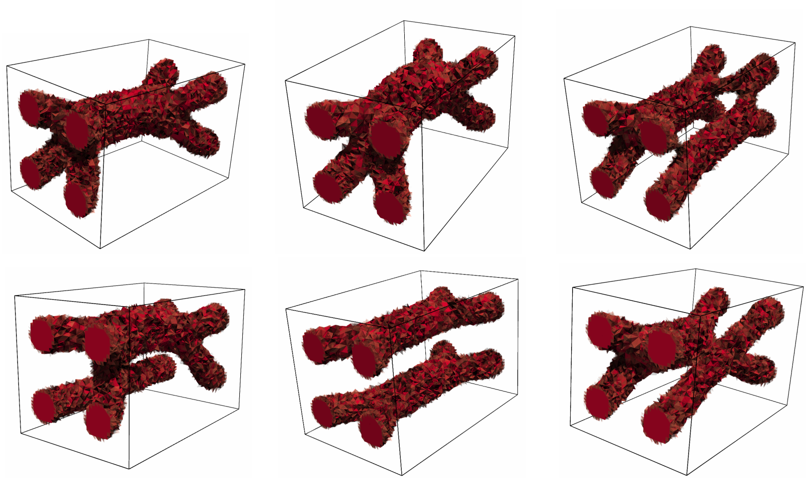

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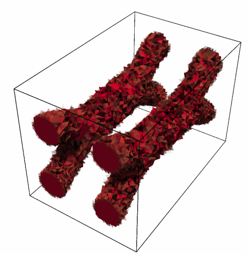
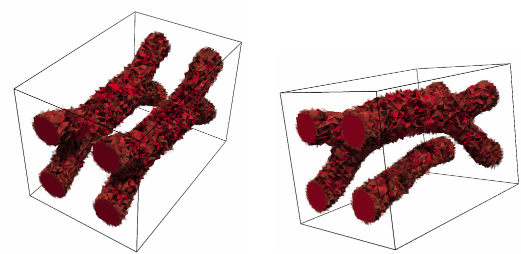


3D five-holes quadruple-pipe



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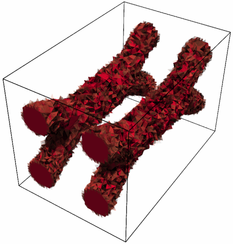
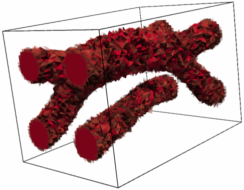
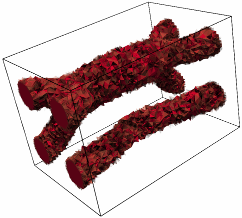

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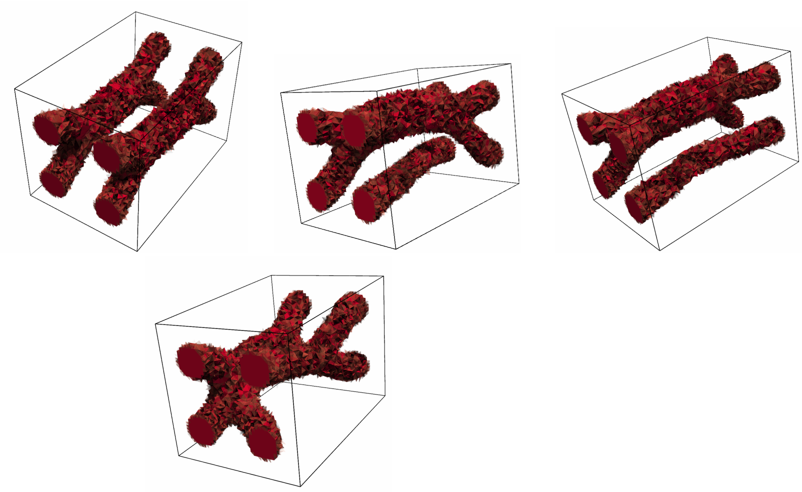

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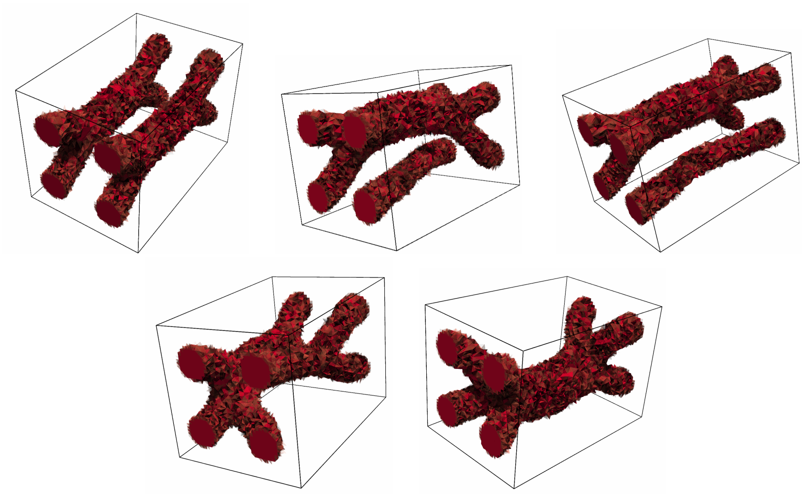
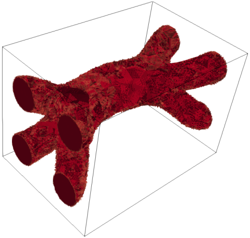


Further refinement



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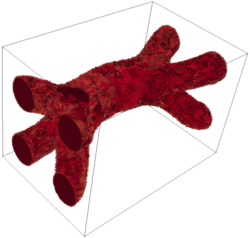

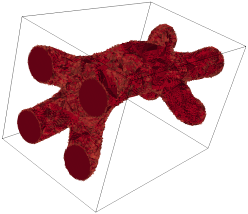

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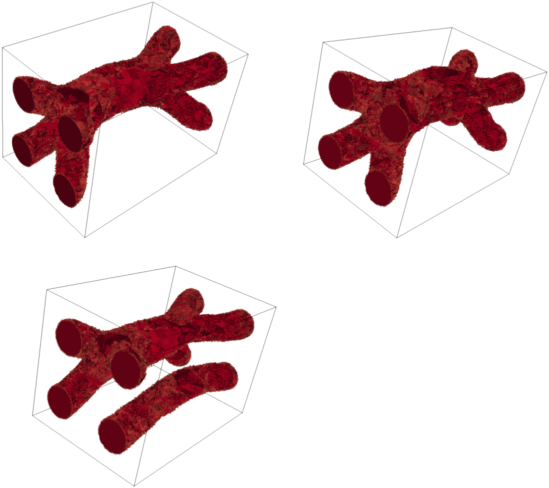

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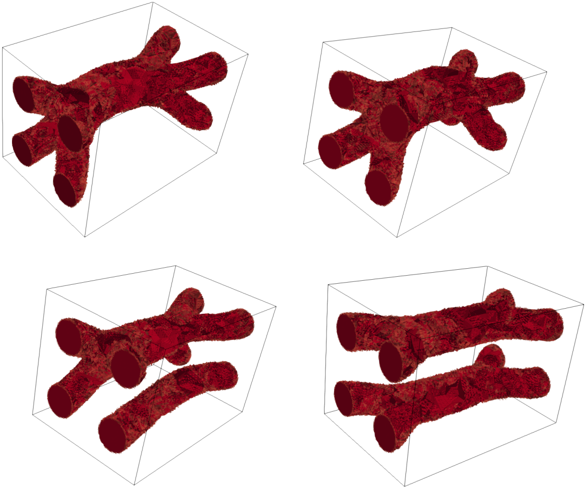

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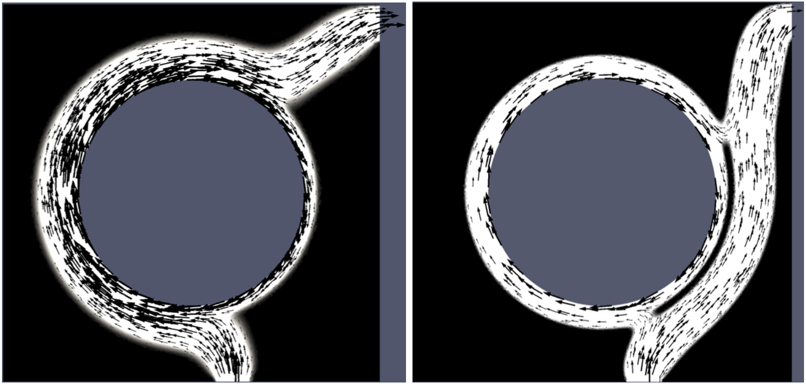
More examples



Roller pump

Compliance of linear elasticity

$$\min_{u,\rho} \int_\Omega f \cdot u \,\mathrm{d}x \quad \text{subject to, for all } v \in H_0^1(\Omega)^d,$$

$$\int_\Omega (\epsilon + (1-\epsilon)\rho^p)[2\mu \nabla_s u : \nabla_s v + \lambda \,\mathrm{div}\, u \cdot \mathrm{div}\, v] - f \cdot v \,\mathrm{d}x = 0,$$

$$0 \leq \rho \leq 1, \quad \int_\Omega \rho \,\mathrm{d}x \leq \gamma |\Omega|.$$

FEM discretization: I. P., *Numer. Math.* (2025)

- Either Sobolev regularization is added or density filtering is used.
- Conforming FEM discretization for (u, ρ).

Then there exists a sequence of discretized solutions to the first-order optimality conditions such that

$$(u_h, \rho_h) \to (u, \rho) \text{ strongly in } H^1(\Omega)^d \times Y,$$

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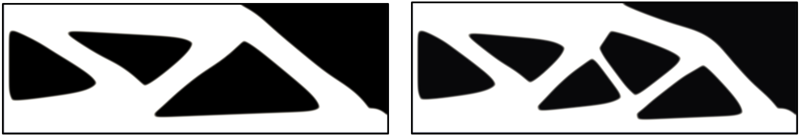

MBB beam

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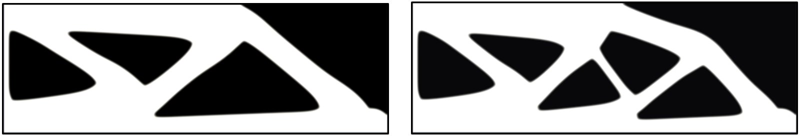

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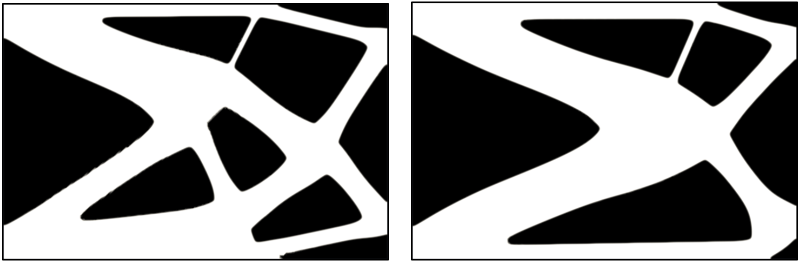

Double cantilever

Preconditioning for Borrvall–Petersson

Need a μ, h, ρ-robust preconditioner.
$\mathrm{DG}_0 \times \mathrm{BDM}_1 \times \mathrm{DG}_0$ discretization for (ρ, u, p).

PDAS linear system: $F'(z)\delta z = -F(z)$

$$\begin{pmatrix} C_\mu & D^\top & 0 \\ D & A_\gamma & B^\top \\ 0 & B & 0 \end{pmatrix} \begin{pmatrix} \delta\boldsymbol{\rho} \\ \delta\mathbf{u} \\ \delta\mathbf{p} \end{pmatrix} = - \begin{pmatrix} \mathbf{f}_\rho \\ \mathbf{f}_u \\ \mathbf{f}_p \end{pmatrix}. \tag{4}$$

$$C_\mu \approx \alpha''(\rho)|u|^2 + \frac{\mu}{(\rho - \epsilon_{\log})^2} + \frac{\mu}{(1 + \epsilon_{\log} - \rho)^2}, \quad D \approx \alpha'(\rho)u,$$

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Solver strategy

- An outer flexible GMRES Krylov method;
- Invert pressure mass matrix M_p (diagonal matrix);
- Invert C_μ (diagonal matrix);
- LU factorize $A_\gamma - DC_\mu^{-1}D^\top$ (expensive).

Can we find a cheaper solve for $A_\gamma - DC_\mu^{-1}D^\top$? ...yes, via a geometric multigrid scheme. It requires a special vertex-star patch smoother and a definition for the active set on the coarser grids.

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Block preconditioning
The Schur complement

$$\begin{pmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{C} & \mathbb{D} \end{pmatrix}^{-1} = \begin{pmatrix} I & -\mathbb{A}^{-1}\mathbb{B} \\ 0 & I \end{pmatrix} \begin{pmatrix} \mathbb{A}^{-1} & 0 \\ 0 & \mathbb{S}^{-1} \end{pmatrix} \begin{pmatrix} I & 0 \\ -\mathbb{C}\mathbb{A}^{-1} & I \end{pmatrix}$$

where the Schur complement is $\mathbb{S} = \mathbb{D} - \mathbb{C}\mathbb{A}^{-1}\mathbb{B}$.

First Schur complement factorization

$$\left(\begin{array}{c|cc} C_\mu & D^\top & 0 \\ \hline D & A_\gamma & B^\top \\ 0 & B & 0 \end{array}\right)$$

$\mathbb{A} = C_\mu \rightarrow$ diagonal

$$\mathbb{S} = S_{1,\gamma} := \begin{pmatrix} A_\gamma - DC_\mu^{-1}D^\top & B^\top \\ B & 0 \end{pmatrix}$$

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$$S_{1,\gamma} = \left(\begin{array}{c|c} A_\gamma - DC_\mu^{-1}D^\top & B^\top \\ \hline B & 0 \end{array}\right)$$

just do another inner block factorization!

Second Schur complement factorization

$$\mathbb{A} = A_\gamma - DC_\mu^{-1}D^\top$$

$$\mathbb{S} = S_{2,\gamma} := -B(A_\gamma - DC_\mu^{-1}D^\top)^{-1}B^\top \underbrace{\to}_{\text{spectrally}} -\gamma^{-1}M_p \text{ as } \gamma \to \infty.$$

Asymptotic spectral equivalence

We can efficiently invert $S_{2,\gamma}$ via GMRES preconditioned with $\gamma^{-1}M_p$.

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Solver diagram

- Primal-dual active-set strategy
  - Krylov solver (FGMRES)
    - Block preconditioner w.r.t. $\mathbb{R}$-block
      - Invert 1×1 Schur complement
      - Solve density-momentum-pressure block

- Solve density-momentum-pressure block
  - Block preconditioner w.r.t. augmented momentum-pressure block
    - Exact inverse of diagonal density block C_μ
    - Exact Schur complement S_{1,γ_d}
      - Block preconditioner w.r.t. pressure block
        - Solve $A_{\gamma_d} - DC_\mu^{-1}D^\top$
        - $\gamma_d M_p^{-1}$ for approximate Schur complement inverse S_{2,γ_d}^{-1}

- Solve $A_{\gamma_d} - DC_\mu^{-1}D^\top$
  - Krylov solver (FGMRES)
    - Full multigrid cycle
      - Coarse-grid solver
        - LU factorization
      - Prolongation operator
        - Standard operator
      - Relaxation
        - GMRES
          - Additive star iteration

Conclusions

- A strategy for computing multiple solutions of topology optimization problems.
- Barrier-like terms + active set strategy + deflation.
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Software

Deflated barrier method

https://github.com/ioannisPApapadopoulos/fir3dab.

Deflation

https://github.com/ioannisPApapadopoulos/Deflation.

Deflation for bifurcation diagrams

https://bitbucket.org/pefarrell/defcon.

Thank you for listening!

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