

24 July 2023

Computing multiple solutions of topology optimization problems

USNCCM17











Thomas Surowiec³

Endre Süli²

¹Imperial College London; ²University of Oxford; ³Simula Research Institute

Topology optimization

Imperial College London

Objective

Find the optimal distribution of a continuum that minimizes a problem-specific cost functional with no prior knowledge of the optimal shape or topology.





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

Models for topology optimization problems tend to:

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

Topology optimization

Imperial College London

Objective

Find the optimal distribution of a continuum that minimizes a problem-specific cost functional with no prior knowledge of the optimal shape or topology.





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

Models for topology optimization problems tend to:

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

Imperial College London

Observations

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

Consequences

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

Our proposal

Observations

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

Consequences

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

Our proposal

Observations

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

Consequences

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

Our proposal

Imperial College London

Observations

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

Consequences

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

Our proposal

Imperial College London

Observations

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

Consequences

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

Our proposal

Imperial College London

Observations

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

Consequences

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

Our proposal

Imperial College London

Deflated barrier method

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





Deflated barrier method

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



Step I: optimize from initial guess



Deflated barrier method

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



Step II: deflate solution found

Imperial College London

Deflated barrier method

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



Step I: optimize from initial guess



Deflated barrier method

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



Step II: deflate solution found



Deflated barrier method

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



Step III: termination on nonconvergence

Construction of deflated problems

A nonlinear transformation of first-order optimality conditions

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

A deflation operator

We say that $\mathcal{M}(z; r)$ is a deflation operator if for any sequence $z \to r$ $\liminf \|\mathcal{G}(z)\| = \liminf \|\mathcal{M}(z; r)\mathcal{F}(z)\| > 0.$

Theorem

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

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

Construction of deflated problems

Imperial College London

A nonlinear transformation of first-order optimality conditions

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

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 $p \ge 1$:

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

Construction of deflated problems

Imperial College London

A nonlinear transformation of first-order optimality conditions

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

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 $p \ge 1$:

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

Imperial College London

Step 1

Compute the normal *undeflated* Newton update δz .

Step 2

Let $m = m(z_k) = \mathcal{M}(z_k, r)$. Then the deflated Newton update is

$$\delta z_D = \tau(z_k, \delta z) \delta z$$

$$\tau(z_k, \delta z) \coloneqq \left(1 + \frac{m^{-1}(m')(\delta z)}{1 - m^{-1}(m')(\delta z)}\right)$$

Imperial College London

Step 1

Compute the normal *undeflated* Newton update δz .

Step 2

Let $m = m(z_k) = \mathcal{M}(z_k, r)$. Then the deflated Newton update is

$$\delta z_{D} = \tau(z_{k}, \delta z) \delta z$$

$$\tau(z_k, \delta z) \coloneqq \left(1 + \frac{m^{-1}(m')(\delta z)}{1 - m^{-1}(m')(\delta z)}\right)$$

Imperial College London

Step 1

Compute the normal *undeflated* Newton update δz .

Step 2

Let $m = m(z_k) = \mathcal{M}(z_k, r)$. Then the deflated Newton update is

$$\delta z_D = \tau(z_k, \delta z) \delta z$$

$$\tau(z_k, \delta z) \coloneqq \left(1 + \frac{m^{-1}(m')(\delta z)}{1 - m^{-1}(m')(\delta z)}\right)$$

Imperial College London

Step 1

Compute the normal *undeflated* Newton update δz .

Step 2

Let $m = m(z_k) = \mathcal{M}(z_k, r)$. Then the deflated Newton update is

$$\delta z_{D} = \tau(z_{k}, \delta z) \delta z$$

$$au(z_k,\delta z)\coloneqq \left(1+rac{m^{-1}(m')(\delta z)}{1-m^{-1}(m')(\delta z)}
ight)$$

Imperial College London



Double-pipe 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.

Imperial College London



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.

Imperial College London



Double-pipe 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.

Imperial College London



Double-pipe 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.

Imperial College London



Double-pipe 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.

Imperial College London



(a) Straight channels

Imperial College London



(a) Straight channels



(b) Double-ended wrench

Imperial College London





(b) Double-ended wrench





Borrvall & Petersson

Imperial College London

Problem

Find velocity u and material distribution ρ 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 $\operatorname{div}(u) = 0$, $0 \le \rho \le 1$, and $\int_{\Omega} \rho \, \mathrm{d}x \le \gamma |\Omega|$.

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

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

Borrvall & Petersson

Imperial College London

Problem

Find velocity u and material distribution ρ 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 $\operatorname{div}(u) = 0$, $0 \le \rho \le 1$, and $\int_{\Omega} \rho \, \mathrm{d}x \le \gamma |\Omega|$.

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

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



Imperial College London



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.







Imperial College London



24 July 2023

Imperial College London























J = 39.67

= 37.3





















J = 54.57

J = 49.93

J = 44.49

J = 41.24















J = 53.25





J = 40.24

J = 38.87

J = 34.07







- 3D discretization on a 40 \times 40 \times 40 block \sim 3,000,000 dofs.
- (Stokes) Nevertheless still numerically tractable via preconditioning techniques implemented with Firedrake 🔮
 - Nested block preconditioning via Schur complements;
 - Augmented Lagrangian control of the pressure Schur complement;
 - Vertex-star patch type relaxation for multigrid schemes.



- 3D discretization on a 40 \times 40 \times 40 block \sim 3,000,000 dofs.
- (Stokes) Nevertheless still numerically tractable via preconditioning techniques implemented with Firedrake 🔮
 - Nested block preconditioning via Schur complements;
 - Augmented Lagrangian control of the pressure Schur complement;
 - Vertex-star patch type relaxation for multigrid schemes.



- 3D discretization on a 40 \times 40 \times 40 block \sim 3,000,000 dofs.
- (Stokes) Nevertheless still numerically tractable via preconditioning techniques implemented with Firedrake
 - Nested block preconditioning via Schur complements;
 - Augmented Lagrangian control of the pressure Schur complement;
 - Vertex-star patch type relaxation for multigrid schemes.



- 3D discretization on a 40 \times 40 \times 40 block \sim 3,000,000 dofs.
- (Stokes) Nevertheless still numerically tractable via preconditioning techniques implemented with Firedrake
 - Nested block preconditioning via Schur complements;
 - Augmented Lagrangian control of the pressure Schur complement;
 - Vertex-star patch type relaxation for multigrid schemes.































Imperial College London



Imperial College London



Imperial College London



Imperial College London



More examples

Imperial College London



Roller pump

More examples







MBB beam

More examples

Imperial College London



Double cantilever

Imperial College London

- A strategy for computing multiple solutions of topology optimization problems.
- Barrier-like terms + active set strategy + deflation.
- Can solve large 3D problems with good preconditioners.

Computing multiple solutions of topology optimization problems.

SIAM Journal on Scientific Computing, 43(3) A1555-A1582, 2021. https://doi.org/10.1137/20M1326209.

Preconditioners for computing multiple solutions in three-dimensional fluid topology optimization

To appear in the SIAM Journal on Scientific Computing, 2023, https://arxiv.org/abs/2202.08248.

Numerical analysis of a topology optimization problem for Stokes flow

Journal of Computational and Applied Mathematics, 412 114295, 2022. https://doi.org/10.1016/j.cam.2022.114295.

Imperial College London

- A strategy for computing multiple solutions of topology optimization problems.
- Barrier-like terms + active set strategy + deflation.
- Can solve large 3D problems with good preconditioners.

Computing multiple solutions of topology optimization problems

SIAM Journal on Scientific Computing, 43(3) A1555-A1582, 2021. https://doi.org/10.1137/20M1326209.

Preconditioners for computing multiple solutions in three-dimensional fluid topology optimization

To appear in the SIAM Journal on Scientific Computing, 2023, https://arxiv.org/abs/2202.08248.

Numerical analysis of a topology optimization problem for Stokes flow

Journal of Computational and Applied Mathematics, 412 114295, 2022. https://doi.org/10.1016/j.cam.2022.114295.

Imperial College London

- A strategy for computing multiple solutions of topology optimization problems.
- Barrier-like terms + active set strategy + deflation.
- Can solve large 3D problems with good preconditioners.

Computing multiple solutions of topology optimization problems

SIAM Journal on Scientific Computing, 43(3) A1555-A1582, 2021. https://doi.org/10.1137/20M1326209.

Preconditioners for computing multiple solutions in three-dimensional fluid topology optimization

To appear in the SIAM Journal on Scientific Computing, 2023, https://arxiv.org/abs/2202.08248.

Numerical analysis of a topology optimization problem for Stokes flow

Journal of Computational and Applied Mathematics, 412 114295, 2022. https://doi.org/10.1016/j.cam.2022.114295.

Imperial College London

- A strategy for computing multiple solutions of topology optimization problems.
- Barrier-like terms + active set strategy + deflation.
- Can solve large 3D problems with good preconditioners.

Computing multiple solutions of topology optimization problems

SIAM Journal on Scientific Computing, 43(3) A1555-A1582, 2021. https://doi.org/10.1137/20M1326209.

Preconditioners for computing multiple solutions in three-dimensional fluid topology optimization

To appear in the SIAM Journal on Scientific Computing, 2023, https://arxiv.org/abs/2202.08248.

Numerical analysis of a topology optimization problem for Stokes flow

Journal of Computational and Applied Mathematics, 412 114295, 2022. https://doi.org/10.1016/j.cam.2022.114295.

Imperial College London

- A strategy for computing multiple solutions of topology optimization problems.
- Barrier-like terms + active set strategy + deflation.
- Can solve large 3D problems with good preconditioners.

Computing multiple solutions of topology optimization problems

SIAM Journal on Scientific Computing, 43(3) A1555-A1582, 2021. https://doi.org/10.1137/20M1326209.

Preconditioners for computing multiple solutions in three-dimensional fluid topology optimization

To appear in the SIAM Journal on Scientific Computing, 2023, https://arxiv.org/abs/2202.08248.

Numerical analysis of a topology optimization problem for Stokes flow

Journal of Computational and Applied Mathematics, 412 114295, 2022. https://doi.org/10.1016/j.cam.2022.114295.





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!

⊠ ioannis.papadopoulos13@imperial.ac.uk

