A Nonlinear Trust-Region Framework for PDE-Constrained Optimization Using Adaptive Model Reduction

Matthew J. Zahr

Institute for Computational and Mathematical Engineering
Farhat Research Group
Stanford University

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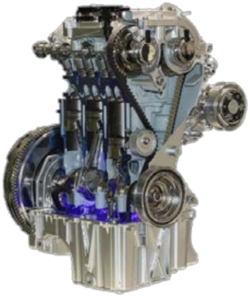
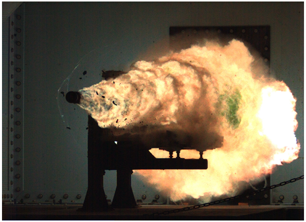
Multiphysics Optimization Key Player in Next-Gen Problems

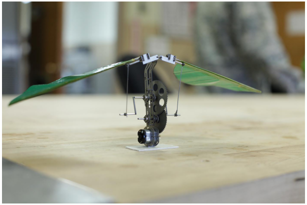
*Current interest in computational physics reaches far beyond analysis of a single configuration of a physical system into **design** (shape and topology[1]), **control**, and **uncertainty quantification***



Engine System



EM Launcher



Micro-Aerial Vehicle

[1] Emergence of additive manufacturing technologies has made topology optimization increasingly relevant.

PDE-Constrained Optimization I

Goal: Rapidly solve PDE-constrained optimization problem of the form

$$\begin{aligned} \underset{\mathbf{u}\in\mathbb{R}^{n_\mathbf{u}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathcal{J}(\mathbf{u},\ \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{r}(\mathbf{u},\ \boldsymbol{\mu}) = 0 \end{aligned}$$

where

- $\mathbf{r} : \mathbb{R}^{n_\mathbf{u}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \to \mathbb{R}^{n_\mathbf{u}}$ is the discretized partial differential equation
- $\mathcal{J} : \mathbb{R}^{n_\mathbf{u}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \to \mathbb{R}$ is the objective function
- $\mathbf{u} \in \mathbb{R}^{n_\mathbf{u}}$ is the PDE state vector
- $\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}$ is the vector of parameters

red indicates a large-scale quantity
blue indicates a small quantity

Projection-Based Model Reduction

- Model Order Reduction (MOR) assumption: *state vector lies in low-dimensional subspace*

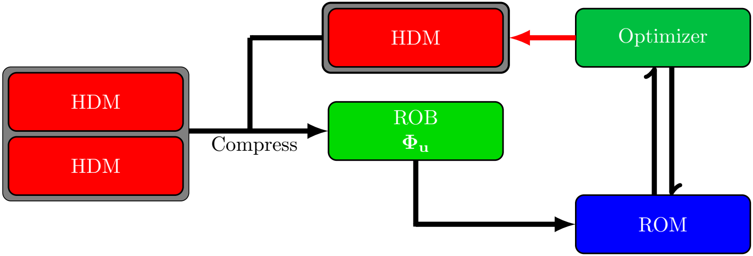
$$\mathbf{u} \approx \mathbf{\Phi}_{\mathbf{u}} \mathbf{u}_r$$

  where
  - $\mathbf{\Phi}_{\mathbf{u}} = \begin{bmatrix} \phi_{\mathbf{u}}^1 & \cdots & \phi_{\mathbf{u}}^{k_{\mathbf{u}}} \end{bmatrix} \in \mathbb{R}^{n_{\mathbf{u}} \times k_{\mathbf{u}}}$ is the reduced basis
  - $\mathbf{u}_r \in \mathbb{R}^{k_{\mathbf{u}}}$ are the reduced coordinates of $\mathbf{u}$
  - $n_{\mathbf{u}} \gg k_{\mathbf{u}}$
- Substitute assumption into High-Dimensional Model (HDM), $\mathbf{r}(\mathbf{u}, \ \boldsymbol{\mu}) = 0$, and apply Galerkin (or Petrov-Galerkin) projection

$$\mathbf{\Phi}_{\mathbf{u}}{}^T \mathbf{r}(\mathbf{\Phi}_{\mathbf{u}} \mathbf{u}_r, \ \boldsymbol{\mu}) = 0$$

- Method of Snapshots and Proper Orthogonal Decomposition used to construct reduced-order basis, $\mathbf{\Phi}_{\mathbf{u}}$

Nonlinear Trust-Region Framework with Adaptive ROMs



[Arian et al., 2000], [Fahl, 2001], [Afanasiev and Hinze, 2001], [Kunisch and Volkwein, 2008], [Hinze and Matthes, 2013], [Yue and Meerbergen, 2013], [Zahr and Farhat, 2014]

Nonlinear Trust-Region Framework with Adaptive ROMs

Nonlinear Trust-Region Framework with Adaptive Model Reduction

- Collect snapshots from HDM at *sparse sampling* of the parameter space
- Build ROB $\boldsymbol{\Phi}_{\mathbf{u}}$ from sparse training
- Solve optimization problem

$$\begin{aligned} \underset{\mathbf{u}_r \in \mathbb{R}^{k_{\mathbf{u}}},\ \boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathcal{J}(\boldsymbol{\Phi}_{\mathbf{u}} \mathbf{u}_r,\ \boldsymbol{\mu}) \\ \text{subject to} \quad & \boldsymbol{\Phi}_{\mathbf{u}}^T \mathbf{r}(\boldsymbol{\Phi}_{\mathbf{u}} \mathbf{u}_r,\ \boldsymbol{\mu}) = 0 \\ & \|\mathbf{r}(\boldsymbol{\Phi}_{\mathbf{u}} \mathbf{u}_r,\ \boldsymbol{\mu})\| \leq \Delta \end{aligned}$$

- Use solution of above problem to enrich training, adapt Δ using standard trust-region methods, and repeat until convergence

PDE-Constrained Optimization II

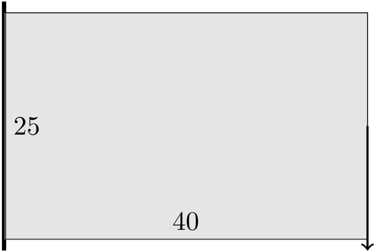
Goal: Rapidly solve PDE-constrained optimization problem of the form

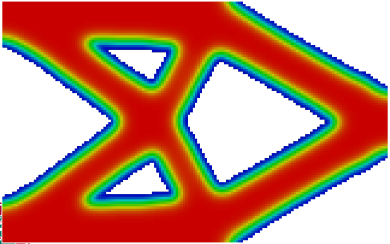
$$\begin{aligned} \underset{\mathbf{u}\in\mathbb{R}^{n_\mathbf{u}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathcal{J}(\mathbf{u},\ \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{r}(\mathbf{u},\ \boldsymbol{\mu}) = 0 \\ & \mathbf{c}(\mathbf{u},\ \boldsymbol{\mu}) \geq 0 \end{aligned}$$

where

- $\mathbf{r} : \mathbb{R}^{n_\mathbf{u}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \to \mathbb{R}^{n_\mathbf{u}}$ is the discretized partial differential equation
- $\mathcal{J} : \mathbb{R}^{n_\mathbf{u}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \to \mathbb{R}$ is the objective function
- $\mathbf{c} : \mathbb{R}^{n_\mathbf{u}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \to \mathbb{R}^{n_\mathbf{c}}$ are the side constraints
- $\mathbf{u} \in \mathbb{R}^{n_\mathbf{u}}$ is the PDE state vector
- $\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}$ is the vector of parameters

Problem Setup





- 16000 8-node brick elements, 77760 dofs
- Total Lagrangian form, finite strain, StVK [2]
- St. Venant-Kirchhoff material
- Sparse Cholesky linear solver (CHOLMOD[3])
- Newton-Raphson nonlinear solver
- Minimum compliance optimization problem

$$
\begin{aligned}
\underset{\mathbf{u}\in\mathbb{R}^{n_{\mathbf{u}}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathbf{f_{ext}}^T\mathbf{u} \\
\text{subject to} \quad & V(\boldsymbol{\mu}) \leq \frac{1}{2}V_0 \\
& \mathbf{r}(\mathbf{u},\ \boldsymbol{\mu}) = 0
\end{aligned}
$$

- Gradient computations: Adjoint method
- Optimizer: SNOPT [Gill et al., 2002]

[2] [Bonet and Wood, 1997, Belytschko et al., 2000]
[3] [Chen et al., 2008]

Restrict Parameter Space to Low-Dimensional Subspace

- *Restrict parameter to a low-dimensional subspace*

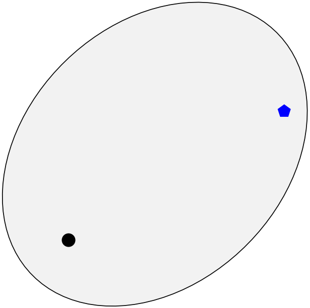
$$\boldsymbol{\mu} \approx \boldsymbol{\Phi}_{\boldsymbol{\mu}} \boldsymbol{\mu}_r$$

  - $\boldsymbol{\Phi}_{\boldsymbol{\mu}} = \begin{bmatrix} \boldsymbol{\phi}_{\boldsymbol{\mu}}^1 & \cdots & \boldsymbol{\phi}_{\boldsymbol{\mu}}^{k_{\boldsymbol{\mu}}} \end{bmatrix} \in \mathbb{R}^{n_{\boldsymbol{\mu}} \times k_{\boldsymbol{\mu}}}$ is the reduced basis
  - $\boldsymbol{\mu}_r \in \mathbb{R}^{k_{\boldsymbol{\mu}}}$ are the reduced coordinates of $\boldsymbol{\mu}$
  - $n_{\boldsymbol{\mu}} \gg k_{\boldsymbol{\mu}}$
- Substitute restriction into reduced-order model to obtain

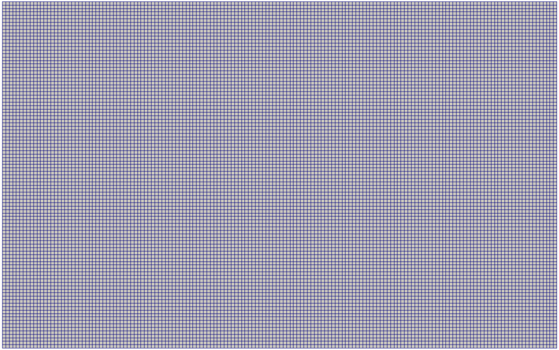
$$\boldsymbol{\Phi}_{\mathbf{u}}{}^T \mathbf{r}(\boldsymbol{\Phi}_{\mathbf{u}} \mathbf{u}_r, \ \boldsymbol{\Phi}_{\boldsymbol{\mu}} \boldsymbol{\mu}_r) = 0$$

- Related work:
  [Maute and Ramm, 1995, Lieberman et al., 2010, Constantine et al., 2014]

Restrict Parameter Space to Low-Dimensional Subspace

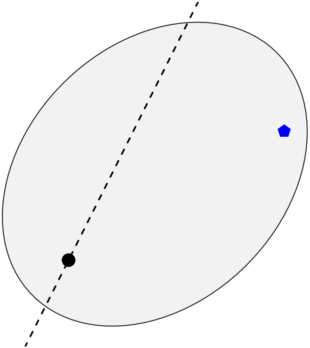


Parameter space

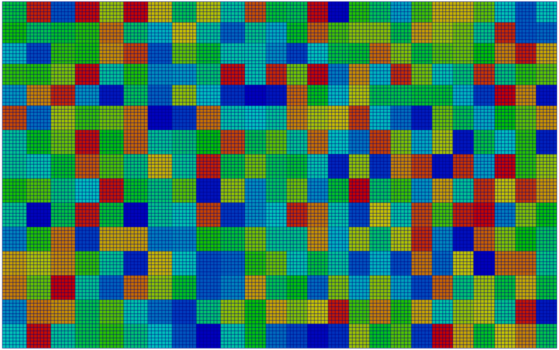


Background mesh

Restrict Parameter Space to Low-Dimensional Subspace



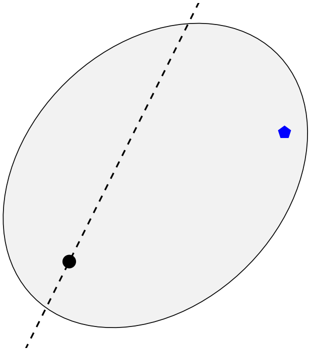
Parameter space



Macroelements

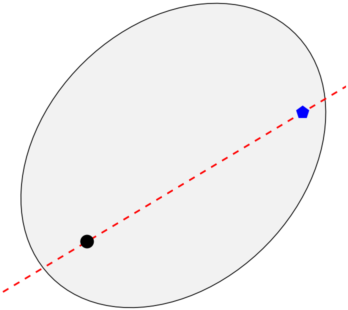
Optimality Conditions to Adapt Reduced-Order Basis, Φ_μ

- Selection of Φ_μ amounts to a *restriction* of the parameter space



Optimality Conditions to Adapt Reduced-Order Basis, $\mathbf{\Phi}_{\boldsymbol{\mu}}$

- Selection of $\mathbf{\Phi}_{\boldsymbol{\mu}}$ amounts to a *restriction* of the parameter space
- Adaptation of $\mathbf{\Phi}_{\boldsymbol{\mu}}$ should attempt to include the optimal solution in the restricted parameter space, i.e. $\boldsymbol{\mu}^* \in \text{col}(\mathbf{\Phi}_{\boldsymbol{\mu}})$
- Adaptation based on **first-order optimality conditions** of HDM optimization problem



Optimality Conditions to Adapt Reduced-Order Basis, Φ_{μ}

Lagrangian

$$\mathcal{L}(\boldsymbol{\mu},\ \boldsymbol{\lambda}) = \mathcal{J}(\mathbf{u}(\boldsymbol{\mu}),\ \boldsymbol{\mu}) - \boldsymbol{\lambda}^T\mathbf{c}(\mathbf{u}(\boldsymbol{\mu}),\ \boldsymbol{\mu})$$

Karush-Kuhn Tucker (KKT) Conditions[4]

$$\begin{aligned}
\nabla_{\boldsymbol{\mu}}\mathcal{L}(\boldsymbol{\mu},\ \boldsymbol{\lambda}) &= 0\\
\boldsymbol{\lambda} &\geq 0\\
\boldsymbol{\lambda}_i\mathbf{c}_i(\mathbf{u}(\boldsymbol{\mu}),\ \boldsymbol{\mu}) &= 0\\
\mathbf{c}(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu}) &\geq 0
\end{aligned}$$

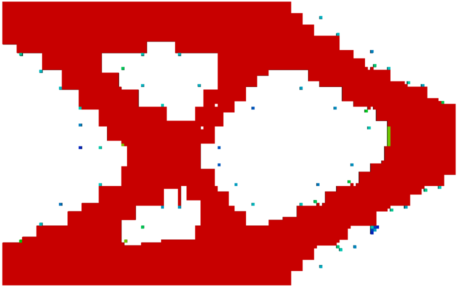
[4] [Nocedal and Wright, 2006]

Lagrangian Gradient Refinement Indicator

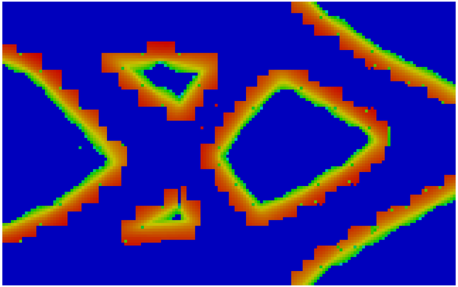
- From Lagrange multiplier estimates, only KKT condition not satisfied automatically:

$$\nabla_{\boldsymbol{\mu}} \mathcal{L}(\boldsymbol{\mu}, \boldsymbol{\lambda}) = 0$$

- Use $|\nabla_{\boldsymbol{\mu}} \mathcal{L}(\boldsymbol{\mu}, \boldsymbol{\lambda})|$ as indicator for **refinement** of discretization of $\boldsymbol{\mu}$-space



$\boldsymbol{\mu}$

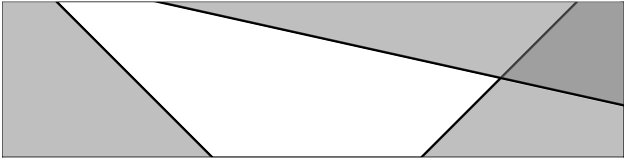


$|\nabla_{\boldsymbol{\mu}} \mathcal{L}(\boldsymbol{\mu}, \boldsymbol{\lambda})|$

Constraints may lead to infeasible sub-problems

Nonlinear Trust-Region MOR [Zahr and Farhat, 2014]

$$\begin{aligned} \underset{\mathbf{u}_r \in \mathbb{R}^{k_{\mathbf{u}}},\ \boldsymbol{\mu}_r \in \mathbb{R}^{k_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathcal{J}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) \\ \text{subject to} \quad & \mathbf{c}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) \geq 0 \\ & \mathbf{r}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) = 0 \\ & ||\mathbf{r}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r)|| \leq \Delta \end{aligned}$$



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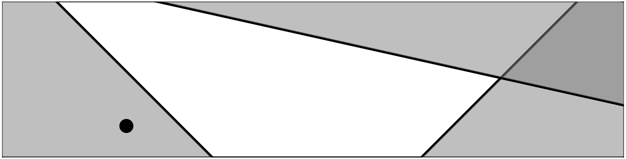

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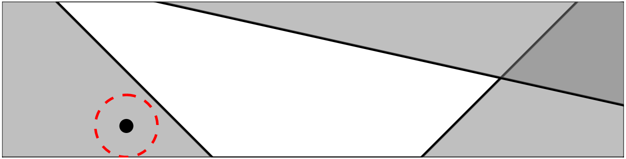
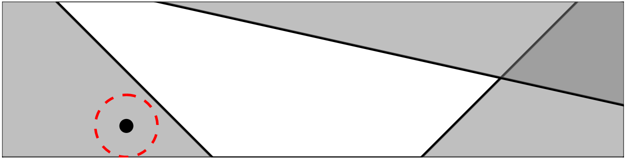


Elastic constraints to circumvent infeasible subproblems

Constrained Nonlinear Trust-Region MOR

$$
\begin{aligned}
\underset{\mathbf{u}_r \in \mathbb{R}^{k_{\mathbf{u}}},\ \boldsymbol{\mu}_r \in \mathbb{R}^{k_{\boldsymbol{\mu}}},\ \mathbf{t} \in \mathbb{R}^{n_{\mathbf{c}}}}{\text{minimize}} \quad & \mathcal{J}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) - \gamma \mathbf{t}^T\mathbf{1} \\
\text{subject to} \quad & \mathbf{c}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) \geq \mathbf{t} \\
& \mathbf{r}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) = 0 \\
& ||\mathbf{r}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r)|| \leq \Delta \\
& \mathbf{t} \leq 0
\end{aligned}
$$



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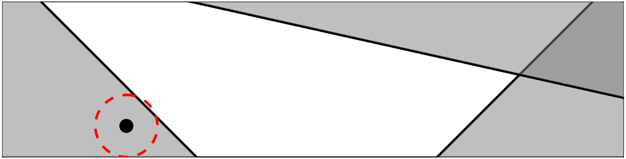

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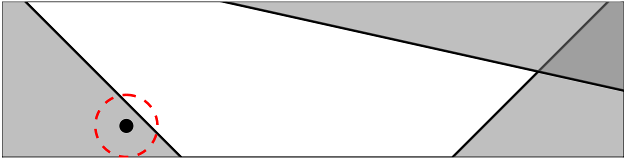

Elastic constraints to circumvent infeasible subproblems

Constrained Nonlinear Trust-Region MOR

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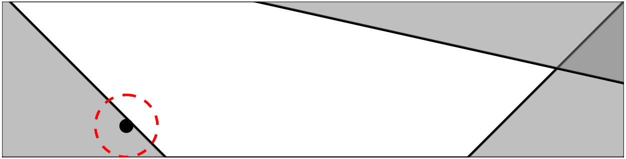

Elastic constraints to circumvent infeasible subproblems

Constrained Nonlinear Trust-Region MOR

$$\begin{aligned}
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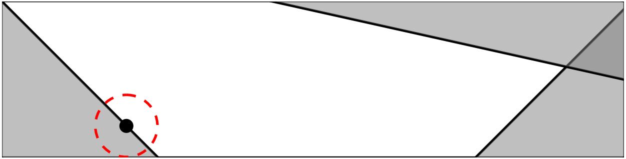
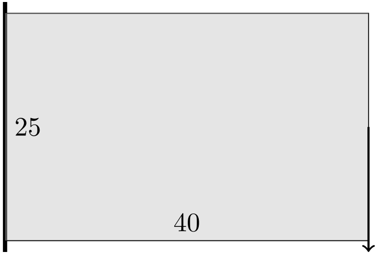
\text{subject to} \quad & \mathbf{c}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) \geq \mathbf{t} \\
& \mathbf{r}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) = 0 \\
& ||\mathbf{r}(\boldsymbol{\Phi}_{\mathbf{u}}\mathbf{u}_r,\ \boldsymbol{\Phi}_{\boldsymbol{\mu}}\boldsymbol{\mu}_r)|| \leq \Delta \\
& \mathbf{t} \leq 0
\end{aligned}$$



Compliance Minimization: 2D Cantilever



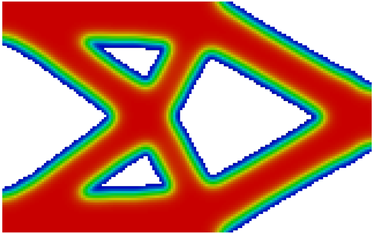
- 16000 8-node brick elements, 77760 dofs
- Total Lagrangian form, finite strain, StVK[5]
- St. Venant-Kirchhoff material
- Sparse Cholesky linear solver (CHOLMOD[6])
- Newton-Raphson nonlinear solver
- Minimum compliance optimization problem

$$\begin{aligned} \underset{\mathbf{u}\in\mathbb{R}^{n_{\mathbf{u}}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathbf{f_{\text{ext}}}^T\mathbf{u} \\ \text{subject to} \quad & V(\boldsymbol{\mu}) \leq \frac{1}{2}V_0 \\ & \mathbf{r}(\mathbf{u},\ \boldsymbol{\mu}) = 0 \end{aligned}$$

- Gradient computations: Adjoint method
- Optimizer: SNOPT [Gill et al., 2002]
- Maximum ROM size: $k_{\mathbf{u}} \leq 5$

[5] [Bonet and Wood, 1997, Belytschko et al., 2000]
[6] [Chen et al., 2008]

Order of Magnitude Speedup to Suboptimal Solution



HDM

CNLTR-MOR + Φ_μ adaptivity

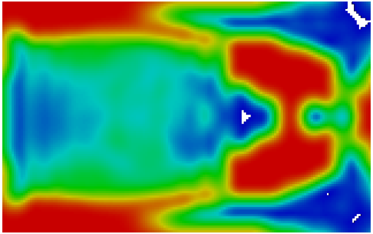
HDM Solution	**HDM** Gradient	**HDM** Optimization
7458s (450)	4018s (411)	8284s

HDM
Elapsed time = 19761s

HDM Solution	**HDM** Gradient	**ROB** Construction	**ROM** Optimization
1049s (64)	88s (9)	727s (56)	39s (3676)

CNLTR-MOR + Φ_μ adaptivity
Elapsed time = 2197s, Speedup ≈ 9x

Better Solution after 64 HDM Evaluations

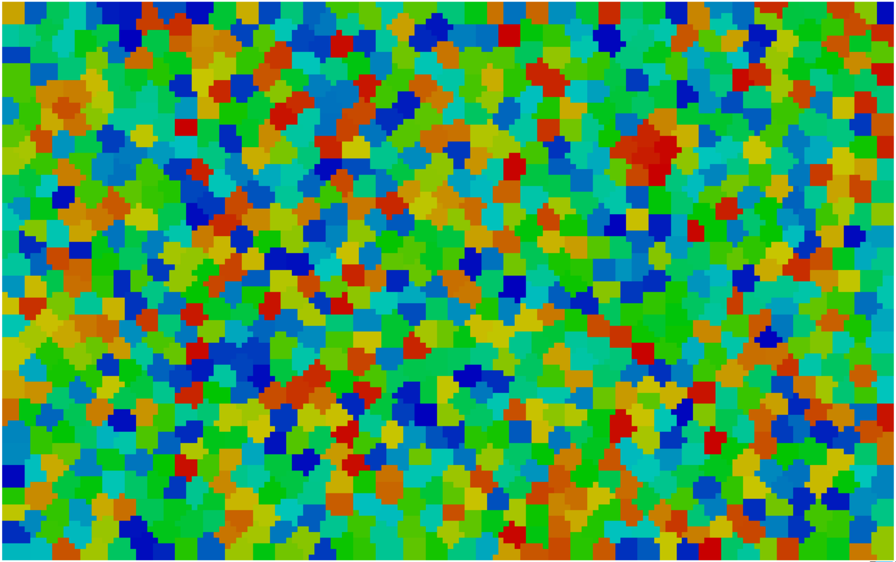


HDM

CNLTR-MOR + Φ_μ adaptivity

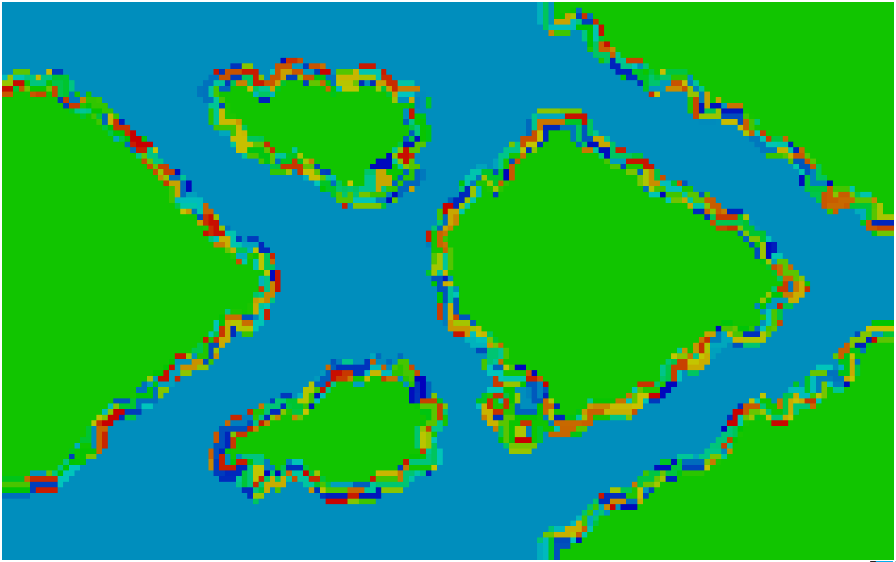
- CNLTR-MOR + Φ_μ adaptivity: superior approximation to optimal solution than HDM approach after fixed number of HDM solves (64)
- Reasonable option to *warm-start* HDM topology optimization

Macro-element Evolution



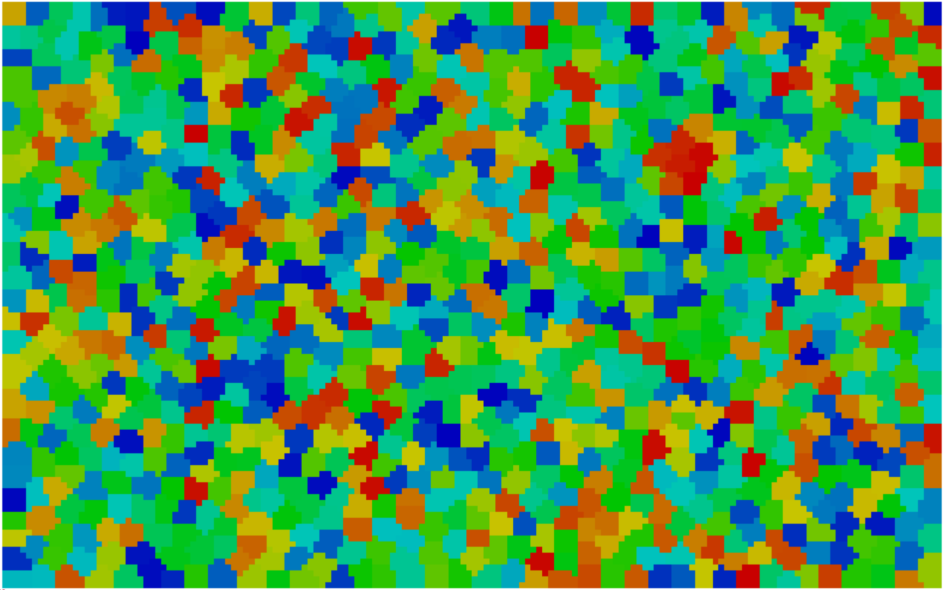
Iteration 0 (1000)

Macro-element Evolution



Iteration 1 (977)

CNLTR-MOR + Φ_μ adaptivity



Summary

- Framework introduced for accelerating PDE-constrained optimization problem with **side constraints** and **large-dimensional parameter space**
- Speedup attained via adaptive reduction of state space and parameter space
- Concepts borrowed from theory of constrained optimization: Lagrangian, KKT system
- Applied to nonlinear topology optimization
  - Order of magnitude speedup speedup observed on 2D and 3D problems
  - Competitive method to warm-start standard topology optimization method

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