

# Accelerating PDE-Constrained Optimization Problems using Adaptive Reduced-Order Models

Matthew J. Zahr

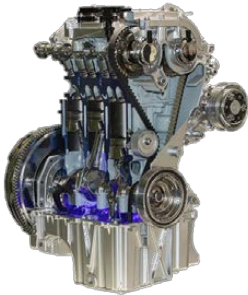
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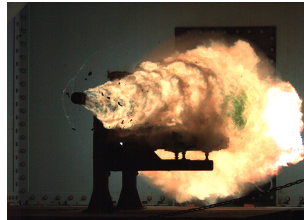


# Multiphysics Optimization Key Player in Next-Gen Problems

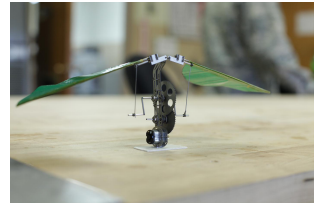
*Current interest in computational physics reaches far beyond analysis of a single configuration of a physical system into **design** (shape and topology<sup>1</sup>), **control**, and **uncertainty quantification***



Engine System



EM Launcher



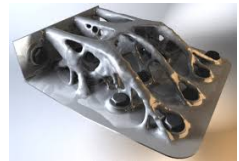
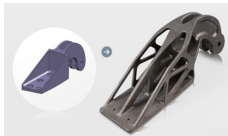
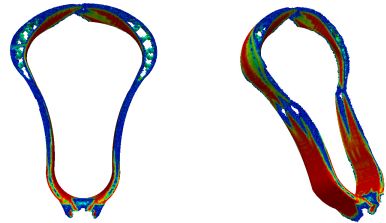
Micro-Aerial Vehicle



<sup>1</sup>Emergence of additive manufacturing technologies has made topology optimization increasingly relevant, particularly in DOE.

# Topology Optimization and Additive Manufacturing<sup>2</sup>

- Emergence of AM has made TO an increasingly relevant topic
- AM+TO lead to highly efficient designs that could not be realized previously
- Challenges: smooth topologies require **very fine** meshes and modeling of complex **manufacturing process**



<sup>2</sup>MIT Technology Review, Top 10 Technological Breakthrough 2013



# PDE-Constrained Optimization I

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

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

where

- $\mathbf{r} : \mathbb{R}^{n_{\mathbf{u}}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \rightarrow \mathbb{R}^{n_{\mathbf{u}}}$  is the discretized partial differential equation
- $\mathcal{J} : \mathbb{R}^{n_{\mathbf{u}}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \rightarrow \mathbb{R}$  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,  $\mathcal{O}(\text{mesh})$*



# Nested Approach to PDE-Constrained Optimization

*Virtually all expense emanates from primal/dual PDE solvers*

Optimizer

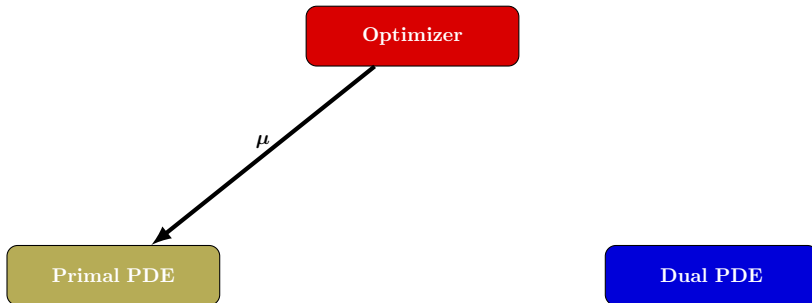
Primal PDE

Dual PDE



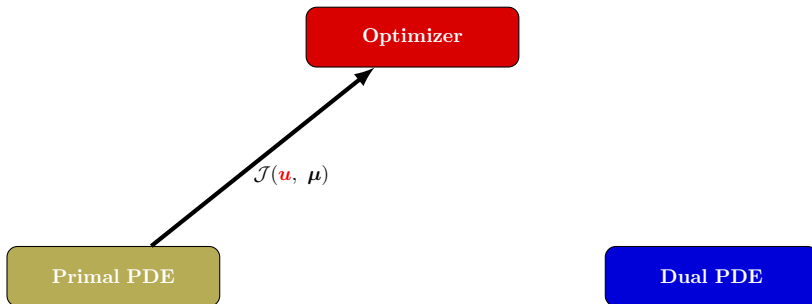
# Nested Approach to PDE-Constrained Optimization

*Virtually all expense emanates from primal/dual PDE solvers*



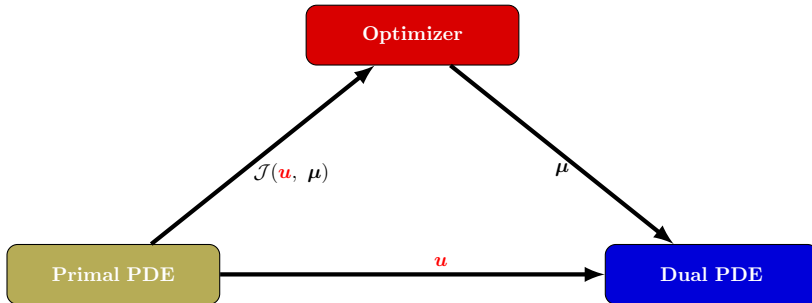
# Nested Approach to PDE-Constrained Optimization

*Virtually all expense emanates from primal/dual PDE solvers*



# Nested Approach to PDE-Constrained Optimization

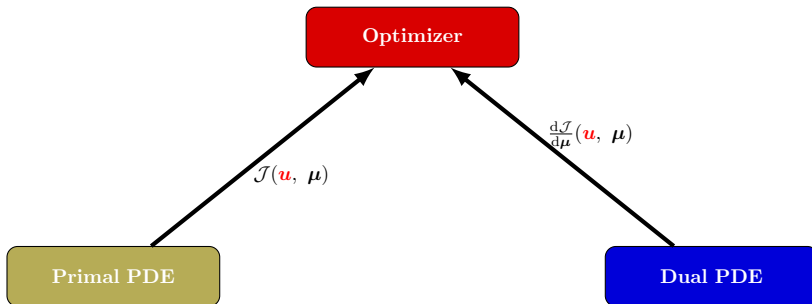
*Virtually all expense emanates from primal/dual PDE solvers*





# Nested Approach to PDE-Constrained Optimization

*Virtually all expense emanates from primal/dual PDE solvers*



# Projection-Based Model Reduction to Reduce PDE Size

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

$$\mathbf{u} \approx \Phi_{\mathbf{u}} \mathbf{u}_r \quad \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} \approx \Phi_{\mathbf{u}} \frac{\partial \mathbf{u}_r}{\partial \boldsymbol{\mu}}$$

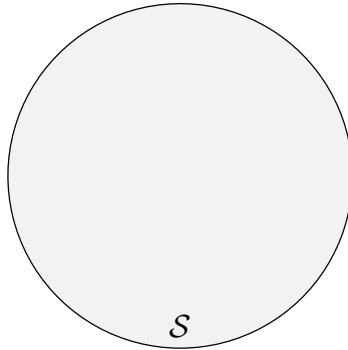
where

- $\Phi_{\mathbf{u}} = [\phi_{\mathbf{u}}^1 \ \cdots \ \phi_{\mathbf{u}}^{k_{\mathbf{u}}}] \in \mathbb{R}^{n_{\mathbf{u}} \times k_{\mathbf{u}}}$  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 project onto test subspace  $\Psi_{\mathbf{u}} \in \mathbb{R}^{n_{\mathbf{u}} \times k_{\mathbf{u}}}$

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



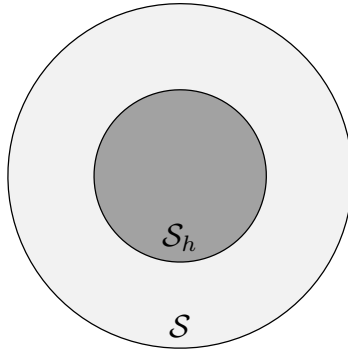
# Connection to Finite Element Method: Hierarchical Subspaces



- $\mathcal{S}$  - infinite-dimensional trial space



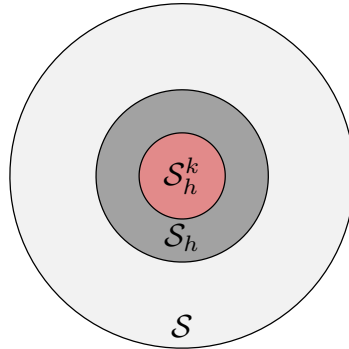
# Connection to Finite Element Method: Hierarchical Subspaces



- $S$  - infinite-dimensional trial space
- $S_h$  - (large) finite-dimensional trial space



# Connection to Finite Element Method: Hierarchical Subspaces



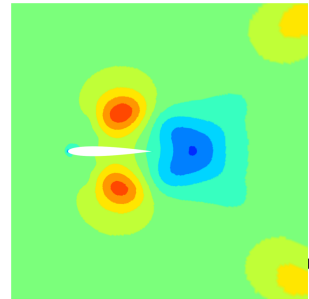
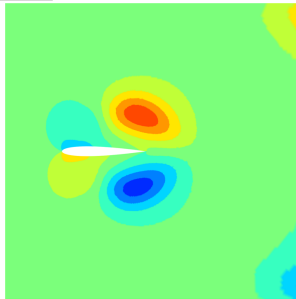
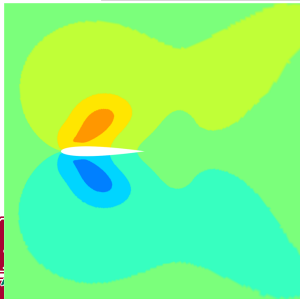
- $S$  - infinite-dimensional trial space
- $S_h$  - (large) finite-dimensional trial space
- $S_h^k$  - (small) finite-dimensional trial space
- $S_h^k \subset S_h \subset S$



# Few Global, Data-Driven Basis Functions v. Many Local Ones



- Instead of using traditional *local* shape functions (e.g., FEM), use *global* shape functions
- Instead of a-priori, analytical shape functions, leverage data-rich computing environment by using *data-driven* modes



# Definition of $\Phi_u$ : Data-Driven Reduction

## State-Sensitivity Proper Orthogonal Decomposition (POD)

- Collect state and sensitivity snapshots by sampling HDM

$$\mathbf{X} = [\mathbf{u}(\mu_1) \quad \mathbf{u}(\mu_2) \quad \cdots \quad \mathbf{u}(\mu_n)]$$

$$\mathbf{Y} = \left[ \frac{\partial \mathbf{u}}{\partial \mu}(\mu_1) \quad \frac{\partial \mathbf{u}}{\partial \mu}(\mu_2) \quad \cdots \quad \frac{\partial \mathbf{u}}{\partial \mu}(\mu_n) \right]$$

- Use Proper Orthogonal Decomposition to generate reduced basis for each individually

$$\Phi_{\mathbf{X}} = \text{POD}(\mathbf{X})$$

$$\Phi_{\mathbf{Y}} = \text{POD}(\mathbf{Y})$$

- Concatenate to get reduced-order basis

$$\Phi_u = [\Phi_{\mathbf{X}} \quad \Phi_{\mathbf{Y}}]$$



# Definition of $\Psi_u$ : Minimum-Residual ROM

Least-Squares Petrov-Galerkin (LSPG)<sup>3</sup> projection

$$\Psi_u = \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \Phi_u$$

## Minimum-Residual Property

A ROM possesses the minimum-residual property if  $\Psi_u \mathbf{r}(\Phi_u \mathbf{u}_r, \boldsymbol{\mu}) = 0$  is equivalent to the optimality condition of  $(\Theta \succ 0)$

$$\underset{\mathbf{u}_r \in \mathbb{R}^{k_u}}{\text{minimize}} \quad \|\mathbf{r}(\Phi_u \mathbf{u}_r, \boldsymbol{\mu})\|_{\Theta}$$

- Implications
  - Recover exact solution when basis not truncated (consistent<sup>3</sup>)
  - Monotonic improvement of solution as basis size increases
  - Ensures sensitivity information in  $\Phi$  cannot degrade state approximation<sup>4</sup>
- LSPG possesses minimum-residual property



<sup>3</sup>[Bui-Thanh et al., 2008]

<sup>4</sup>[Fahl, 2001]





# Definition of $\frac{\partial \mathbf{u}_r}{\partial \mu}$ : Minimum-Residual Reduced Sensitivities

Traditional sensitivity analysis

$$\frac{\partial \mathbf{u}_r}{\partial \mu} = - \left[ \sum_{j=1}^N \mathbf{r}_j \Phi_{\mathbf{u}}^T \frac{\partial \mathbf{r}_j}{\partial \mathbf{u} \partial \mu} \Phi_{\mathbf{u}} + \left( \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \Phi_{\mathbf{u}} \right)^T \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \Phi_{\mathbf{u}} \right]^{-1} \left( \sum_{j=1}^N \mathbf{r}_j \Phi_{\mathbf{u}}^T \frac{\partial^2 \mathbf{r}_j}{\partial \mathbf{u} \partial \mu} + \left( \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \Phi_{\mathbf{u}} \right)^T \frac{\partial \mathbf{r}}{\partial \mu} \right)$$

- + Guaranteed to give rise to *exact* derivatives of ROM quantities of interest
- Requires 2nd derivatives of  $\mathbf{r}$
- $\Phi_{\mathbf{u}} \frac{\partial \mathbf{u}_r}{\partial \mu}$  not guaranteed to be good approximate to full sensitivity  $\frac{\partial \mathbf{u}}{\partial \mu}$



# Definition of $\frac{\partial \mathbf{u}_r}{\partial \boldsymbol{\mu}}$ : Minimum-Residual Reduced Sensitivities

Minimum-residual sensitivity analysis

$$\widehat{\frac{\partial \mathbf{u}_r}{\partial \boldsymbol{\mu}}} = \arg \min_{\mathbf{a}} \|\Phi_{\mathbf{u}} \mathbf{a} - \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}}\|_{\Theta} = - \left[ \left( \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \Phi_{\mathbf{u}} \right)^T \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \Phi_{\mathbf{u}} \right]^{-1} \left( \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \Phi_{\mathbf{u}} \right)^T \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$

- + Minimum-residual property -  $\Phi_{\mathbf{u}} \widehat{\frac{\partial \mathbf{u}_r}{\partial \boldsymbol{\mu}}}$  is  $\Theta$ -optimal solution to  $\frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}}$  in  $\Phi_{\mathbf{u}}$
- + Does not require 2nd derivatives of  $\mathbf{r}$
- $\widehat{\frac{\partial \mathbf{u}_r}{\partial \boldsymbol{\mu}}} \neq \frac{\partial \mathbf{u}_r}{\partial \boldsymbol{\mu}}$ , i.e., it is not the true ROM sensitivity



# Offline-Online Approach to Optimization

Schematic



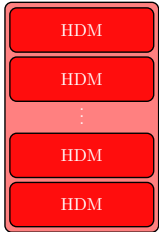
$\mu$ -space



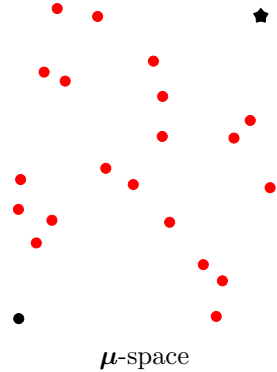
Breakdown of Computational Effort



# Offline-Online Approach to Optimization



Schematic



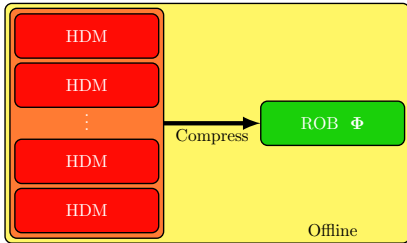
$\mu$ -space



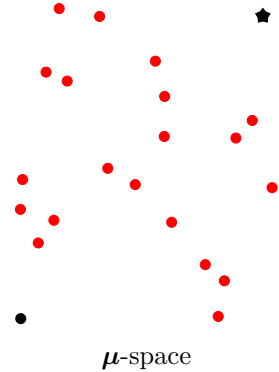
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Schematic



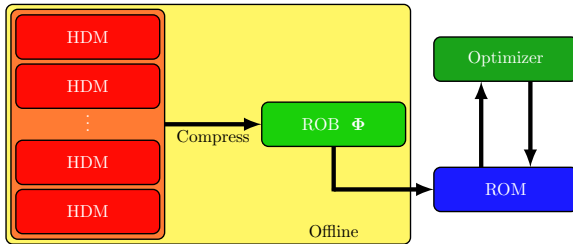
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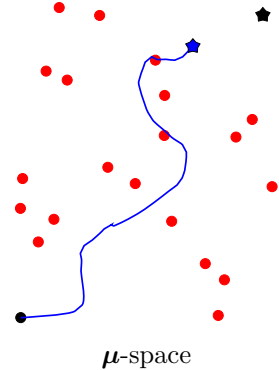
Breakdown of Computational Effort



# Offline-Online Approach to Optimization



Schematic



$\mu$ -space

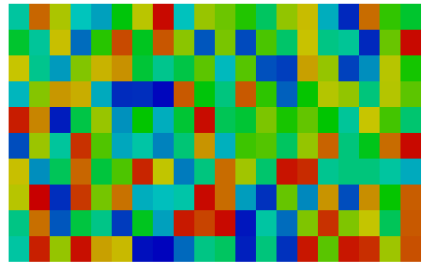


Breakdown of Computational Effort



# Numerical Demonstration: Offline-Online Breakdown

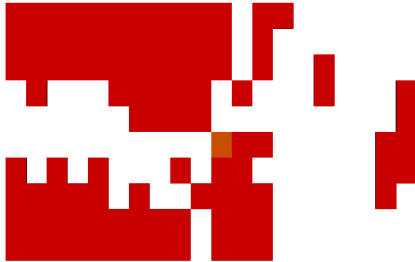
- Parameter reduction ( $\Phi_{\mu}$ )
  - *a priori spatial clustering*
  - $k_{\mu} = 200$
- Greedy Training
  - 5000 candidate points (LHS)
  - 50 snapshots
  - Error indicator:  $\|\mathbf{r}(\Phi_{\mathbf{u}}\mathbf{u}_r, \Phi_{\mu}\boldsymbol{\mu}_r)\|$
- State reduction ( $\Phi_{\mathbf{u}}$ )
  - POD
  - $k_{\mathbf{u}} = 25$
  - Polynomialization acceleration



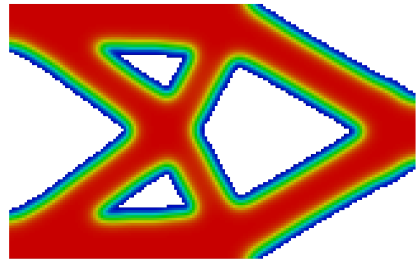
Material Basis



# Numerical Demonstration: Offline-Online Breakdown



Optimal Solution (ROM)



Optimal Solution (HDM)

HDM Solution	ROB Construction	Greedy Algorithm	ROM Optimization
$2.84 \times 10^3$ s	$5.48 \times 10^4$ s	$1.67 \times 10^5$ s	30 s
1.26%	24.36%	74.37%	0.01%



HDM Optimization:  $1.97 \times 10^4$  s





# ROM-Based Trust-Region Framework for Optimization



Schematic



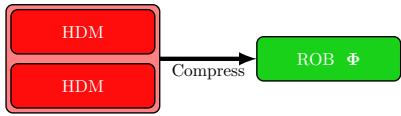
$\mu$ -space



Breakdown of Computational Effort



# ROM-Based Trust-Region Framework for Optimization



Schematic



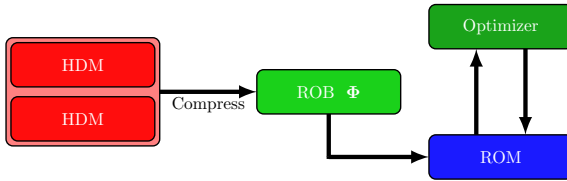
$\mu$ -space



Breakdown of Computational Effort



# ROM-Based Trust-Region Framework for Optimization



Schematic



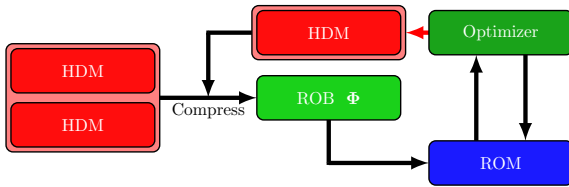
$\mu$ -space



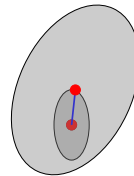
Breakdown of Computational Effort



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Schematic



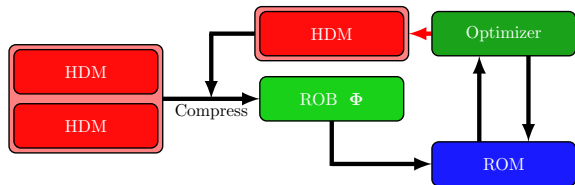
$\mu$ -space



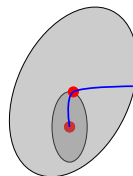
Breakdown of Computational Effort



# ROM-Based Trust-Region Framework for Optimization



Schematic



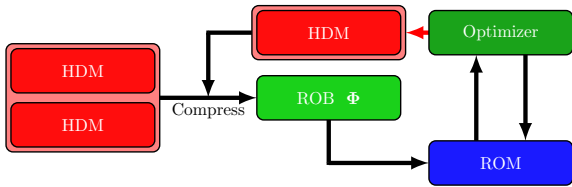
$\mu$ -space



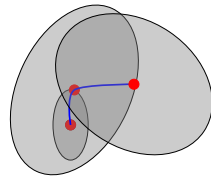
Breakdown of Computational Effort



# ROM-Based Trust-Region Framework for Optimization



Schematic



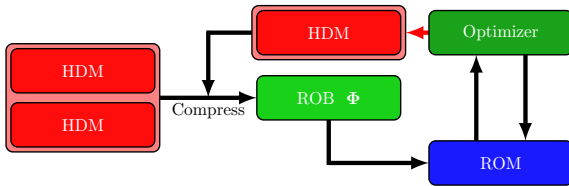
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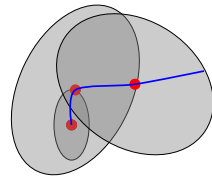
Breakdown of Computational Effort



# ROM-Based Trust-Region Framework for Optimization



Schematic



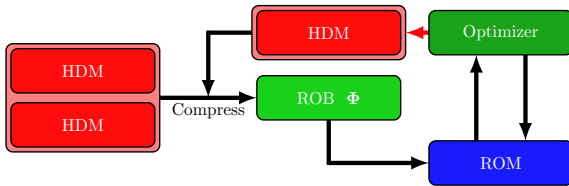
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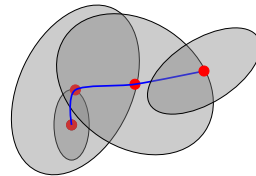
Breakdown of Computational Effort



# ROM-Based Trust-Region Framework for Optimization



Schematic



$\mu$ -space

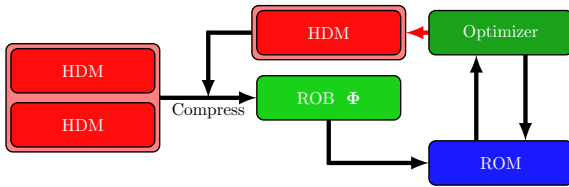


Breakdown of Computational Effort

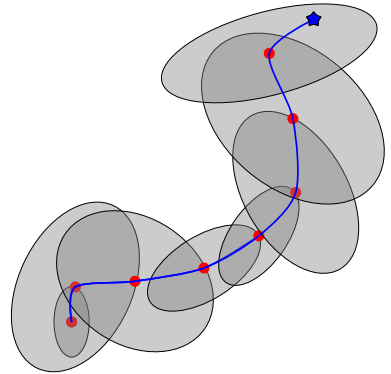




# ROM-Based Trust-Region Framework for Optimization



Schematic



$\mu$ -space



Breakdown of Computational Effort



# ROM-Based Trust-Region Framework for Optimization

## Nonlinear Trust-Region Framework with Adaptive Model Reduction

- Collect snapshots from HDM at *sparse sampling* of the parameter space
- Build ROB  $\Phi_u$  from sparse training
- Solve optimization problem

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

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

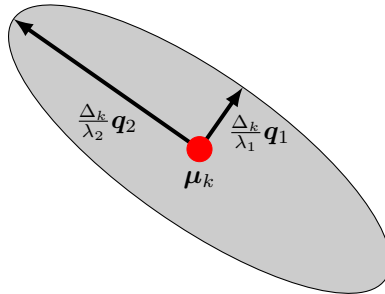


# Residual-Based Trust-Region Interpretation

Let  $\hat{r}(\boldsymbol{\mu}) = \mathbf{r}(\Phi_{\mathbf{u}} \mathbf{u}_r(\boldsymbol{\mu}), \boldsymbol{\mu})$  and  $\mathbf{A}_k = \frac{\partial \hat{r}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_k)^T \frac{\partial \hat{r}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_k) = \mathbf{Q}_k \boldsymbol{\Lambda}_k^2 \mathbf{Q}_k^T$ .

Then, to first order<sup>5</sup>,

$$\|\hat{r}(\boldsymbol{\mu})\|_2 = \left\| \frac{\partial \hat{r}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_k)(\boldsymbol{\mu} - \boldsymbol{\mu}_k) \right\|_2 = \|\boldsymbol{\mu} - \boldsymbol{\mu}_k\|_{\mathbf{A}_k} \leq \Delta_k$$



Annotated schematic of trust-region:  $\mathbf{q}_i = \mathbf{Q}_k \mathbf{e}_i$  and  $\lambda_i = \mathbf{e}_i^T \boldsymbol{\Lambda}_k \mathbf{e}_i$



<sup>5</sup>assuming  $\hat{r}(\boldsymbol{\mu}_k) = 0$ , i.e., ROM exact at trust-region center



# ROM-Based Trust-Region Framework for Optimization

## Ingredients of Proposed Approach [Zahr and Farhat, 2014]

- Minimum-residual ROM (LSPG) and minimum-error sensitivities
  - $\mathcal{J}(\mathbf{u}, \boldsymbol{\mu}) = \mathcal{J}(\Phi_{\mathbf{u}}\mathbf{u}_r, \boldsymbol{\mu})$  and  $\frac{d\mathcal{J}}{d\boldsymbol{\mu}}(\mathbf{u}, \boldsymbol{\mu}) = \frac{d\mathcal{J}}{d\boldsymbol{\mu}}(\Phi_{\mathbf{u}}\mathbf{u}_r, \boldsymbol{\mu})$  for training parameters  $\boldsymbol{\mu}$
- Reduced optimization (sub)problem

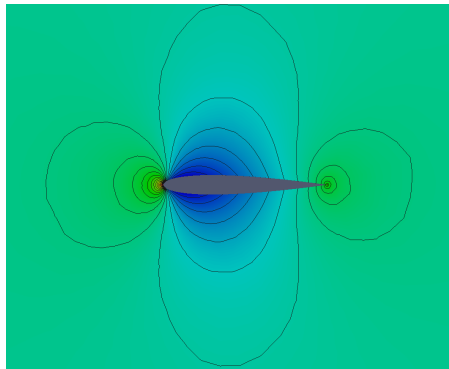
$$\begin{aligned} & \underset{\mathbf{u}_r \in \mathbb{R}^{n_{\mathbf{u}}}, \boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} && \mathcal{J}(\Phi_{\mathbf{u}}\mathbf{u}_r, \boldsymbol{\mu}) \\ & \text{subject to} && \Psi_{\mathbf{u}}^T \mathbf{r}(\Phi_{\mathbf{u}}\mathbf{u}_r, \boldsymbol{\mu}) = 0 \\ & && \|\mathbf{r}(\Phi_{\mathbf{u}}\mathbf{u}_r, \boldsymbol{\mu})\|_2^2 \leq \Delta \end{aligned}$$

- Efficiently update ROB with additional snapshots or new translation vector
  - Without re-computing SVD of entire snapshot matrix
- Adaptive selection of  $\Delta \rightarrow$  trust-region approach

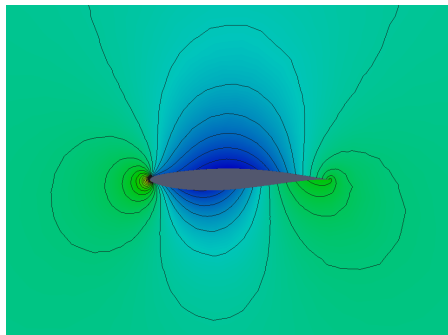


# Compressible, Inviscid Airfoil Inverse Design

Pressure discrepancy minimization (Euler equations)



NACA0012: Initial

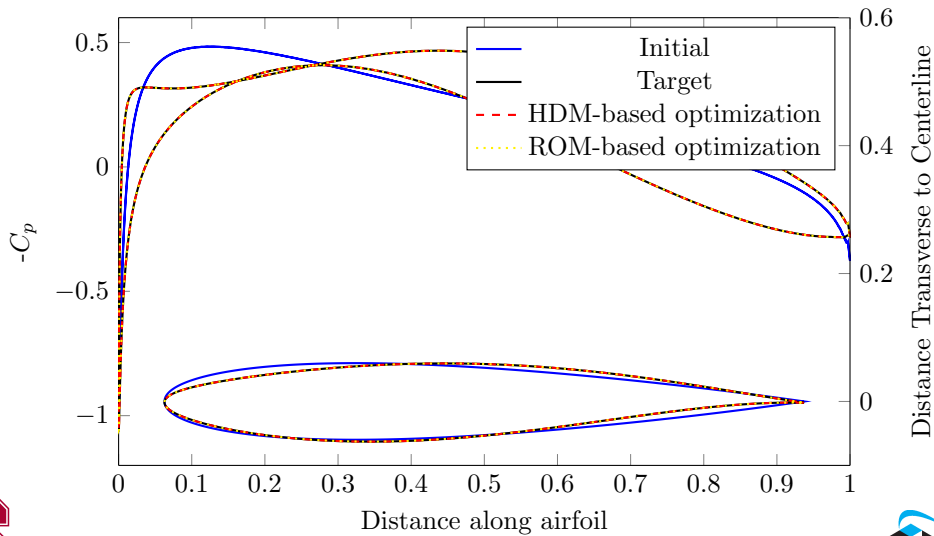


RAE2822: Target

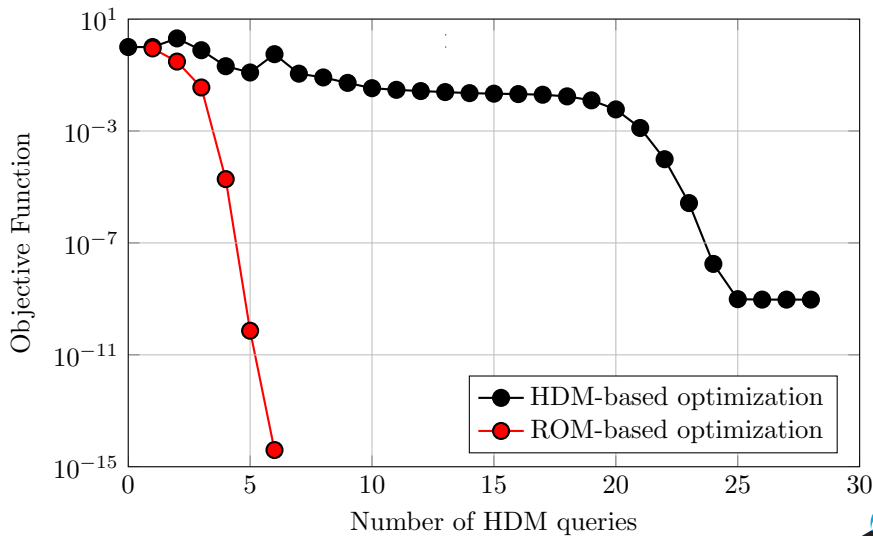
Pressure field for airfoil configurations at  $M_\infty = 0.5$ ,  $\alpha = 0.0^\circ$



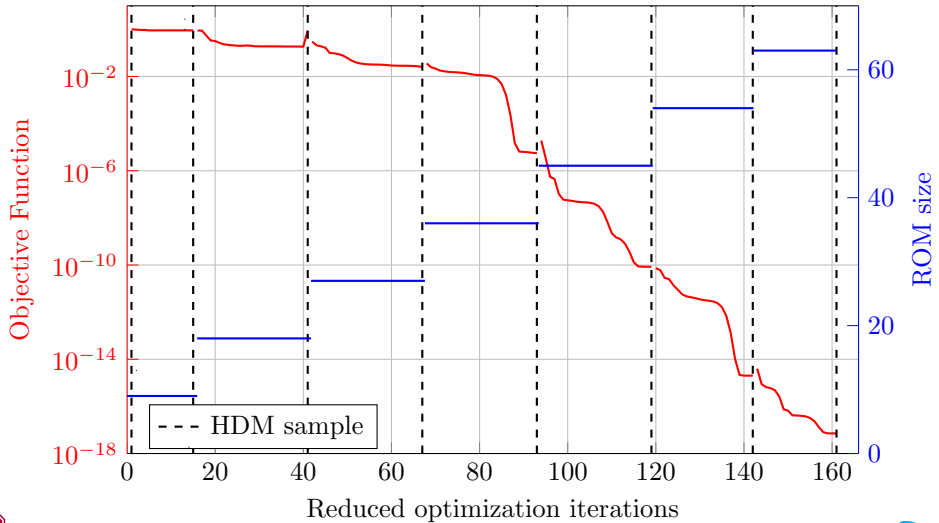
# ROM-Constrained Optimization Solver Recovers Target



# ROM Solver Requires 4× Fewer HDM Queries



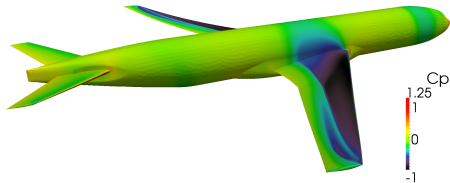
# At the Cost of ROM Queries



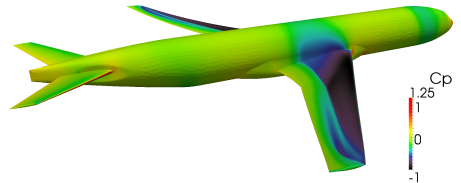


## Next: Shape Optimization of Full Aircraft (CRM)

*ROMs are fast, accurate, and require limited resources*



HDM solution (Drag = 142.336kN)



ROM solution (Drag = 142.304kN)

- HDM:  $70 \times 10^6$  DOF, **2hr on 1024** Intel Xeon E5-2698 v3 cores (2.3GHz)
- ROM: **170s on 2** Intel i7 cores (1.8GHz)
- Relative error in drag 0.022%
- CPU-time speedup greater than  $2.15 \times 10^4$
- Wall-time speedup greater than **42**
- Washabaugh, Zahr, Farhat (AIAA, 2016)



# PDE-Constrained Optimization II

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

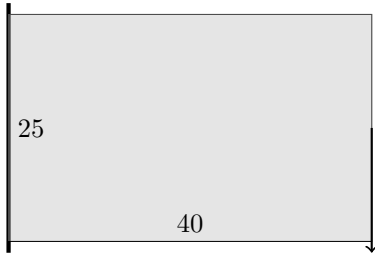
$$\begin{aligned} & \underset{\mathbf{u} \in \mathbb{R}^{n_u}, \boldsymbol{\mu} \in \mathbb{R}^{n_\mu}}{\text{minimize}} && \mathcal{J}(\mathbf{u}, \boldsymbol{\mu}) \\ & \text{subject to} && \mathbf{r}(\mathbf{u}, \boldsymbol{\mu}) = \mathbf{0} \\ & && \mathbf{c}(\mathbf{u}, \boldsymbol{\mu}) \geq \mathbf{0}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

where

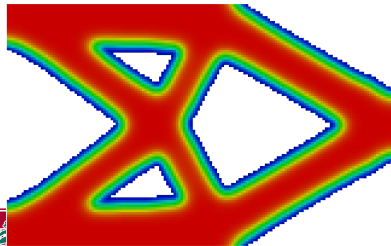
- $\mathbf{r} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \rightarrow \mathbb{R}^{n_u}$  is the discretized partial differential equation
- $\mathcal{J} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \rightarrow \mathbb{R}$  is the objective function
- $\mathbf{c} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu}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



# Problem Setup



- 16000 8-node brick elements, 77760 dofs
- Total Lagrangian form, finite strain, StVK<sup>6</sup>
- St. Venant-Kirchhoff material
- Sparse Cholesky linear solver (CHOLMOD<sup>7</sup>)
- Newton-Raphson nonlinear solver
- Minimum compliance optimization problem



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

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

<sup>6</sup>[Bonet and Wood, 1997, Belytschko et al., 2000]

<sup>7</sup>[Chen et al., 2008]



# Restrict Parameter Space to Low-Dimensional Subspace

- *Restrict parameter to a low-dimensional subspace*

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

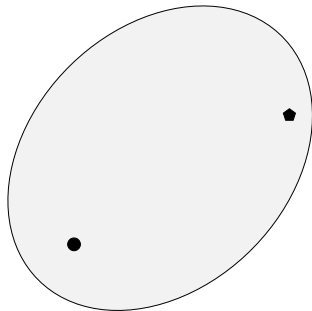
- $\boldsymbol{\Phi}_\mu = \begin{bmatrix} \phi_\mu^1 & \dots & \phi_\mu^{k_\mu} \end{bmatrix} \in \mathbb{R}^{n_\mu \times k_\mu}$  is the reduced basis
- $\boldsymbol{\mu}_r \in \mathbb{R}^{k_\mu}$  are the reduced coordinates of  $\boldsymbol{\mu}$
- $n_\mu \gg k_\mu$
- Substitute restriction into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

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

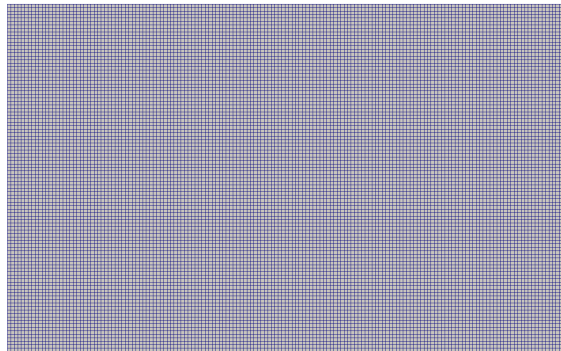
- Related work:  
 [Maute and Ramm, 1995, Lieberman et al., 2010, Constantine et al., 2014]



# Restrict Parameter Space to Low-Dimensional Subspace



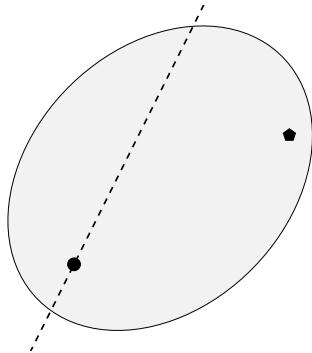
$\mu$ -space



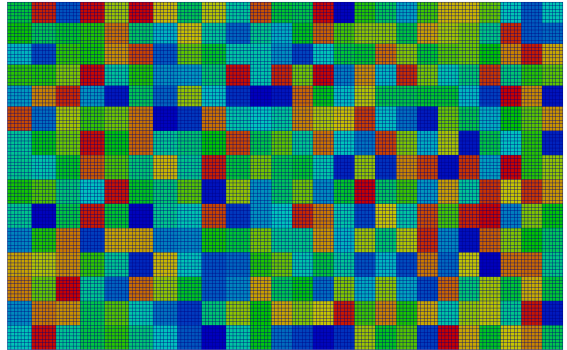
Background mesh



# Restrict Parameter Space to Low-Dimensional Subspace



$\mu$ -space

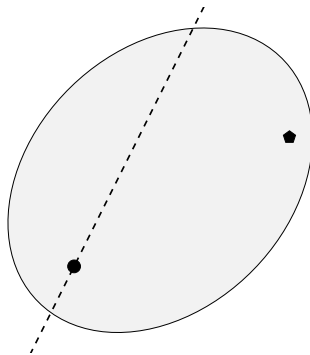


Macroelements



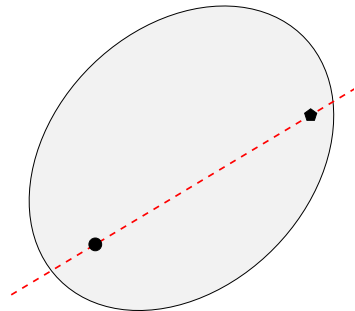
# Optimality Conditions to Adapt Reduced-Order Basis, $\Phi_\mu$

- Selection of  $\Phi_\mu$  amounts to a *restriction* of the parameter space



# Optimality Conditions to Adapt Reduced-Order Basis, $\Phi_\mu$

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





# Optimality Conditions to Adapt Reduced-Order Basis, $\Phi_\mu$

## 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<sup>8</sup>

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

$$\boldsymbol{\lambda} \geq 0$$

$$\lambda_i \mathbf{c}_i(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu}) = 0$$

$$\mathbf{c}(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu}) \geq 0$$



<sup>8</sup>[Nocedal and Wright, 2006]

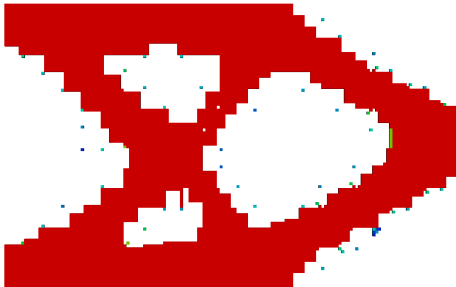


# Lagrangian Gradient Refinement Indicator

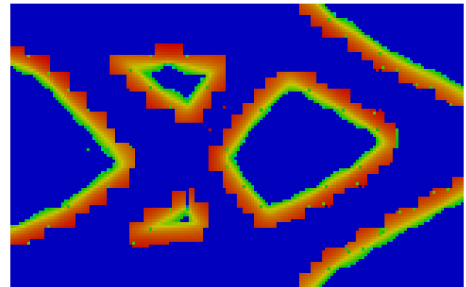
- From Lagrange multiplier estimates, only KKT condition not satisfied automatically:

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

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



$\mu$



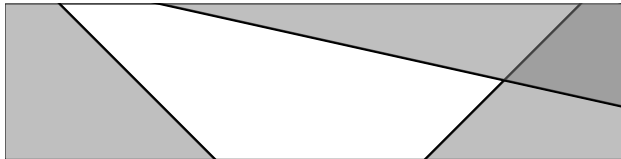
$|\nabla_{\mu} \mathcal{L}(\mu, \lambda)|$



# Constraints may lead to infeasible sub-problems

## Non-Quadratic Trust-Region MOR [Zahr and Farhat, 2014]

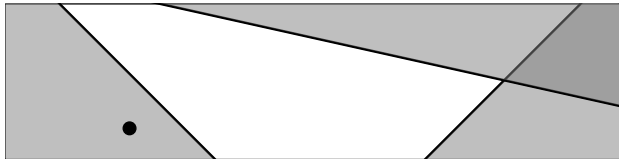
$$\begin{aligned}
 & \text{minimize} && \mathcal{J}(\Phi_u \mathbf{u}_r, \Phi_\mu \boldsymbol{\mu}_r) \\
 & \mathbf{u}_r \in \mathbb{R}^{k_u}, \boldsymbol{\mu}_r \in \mathbb{R}^{k_\mu} \\
 & \text{subject to} && \mathbf{c}(\Phi_u \mathbf{u}_r, \Phi_\mu \boldsymbol{\mu}_r) \geq 0 \\
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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



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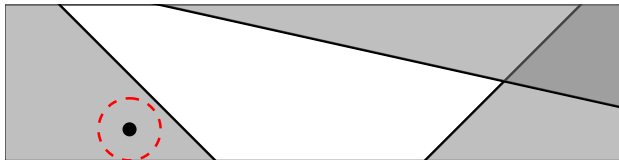
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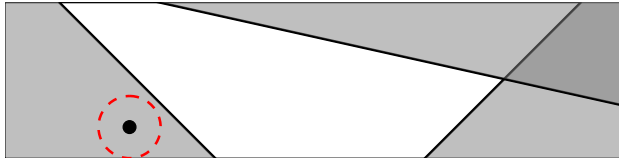
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# Elastic constraints to circumvent infeasible subproblems

## Constrained Non-Quadratic Trust-Region MOR (CNQTR-MOR)

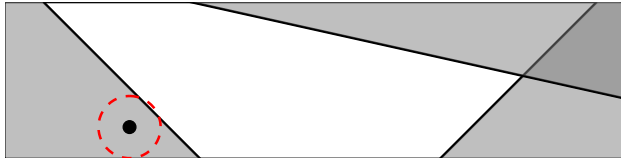
$$\begin{aligned}
 & \text{minimize} && \mathcal{J}(\Phi_u \mathbf{u}_r, \Phi_\mu \boldsymbol{\mu}_r) - \gamma \mathbf{t}^T \mathbf{1} \\
 & \mathbf{u}_r \in \mathbb{R}^{k_u}, \boldsymbol{\mu}_r \in \mathbb{R}^{k_\mu}, \mathbf{t} \in \mathbb{R}^{n_c} \\
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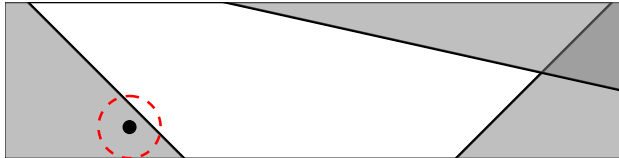
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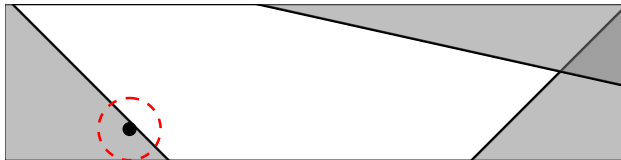




# Elastic constraints to circumvent infeasible subproblems

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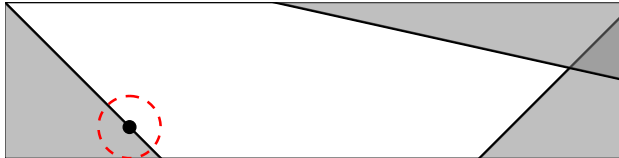
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# Elastic constraints to circumvent infeasible subproblems

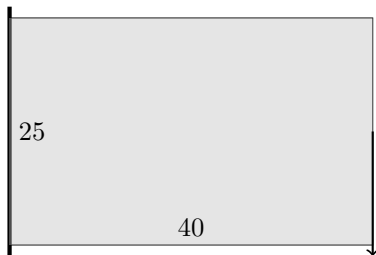
## Constrained Non-Quadratic Trust-Region MOR (CNQTR-MOR)

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 \end{aligned}$$



# Compliance Minimization: 2D Cantilever

- 16000 8-node brick elements, 77760 dofs
- Total Lagrangian form, finite strain, StVK<sup>9</sup>
- St. Venant-Kirchhoff material
- Sparse Cholesky linear solver (CHOLMOD<sup>10</sup>)
- Newton-Raphson nonlinear solver
- Minimum compliance optimization problem



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

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

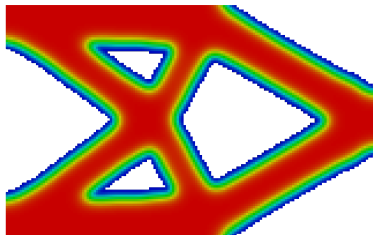


<sup>9</sup>[Bonet and Wood, 1997, Belytschko et al., 2000]

<sup>10</sup>[Chen et al., 2008]



# Order of Magnitude Speedup to Suboptimal Solution



HDM



CNQTR-MOR +  $\Phi_\mu$  adaptivity

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

**HDM**

Elapsed time = 19761s

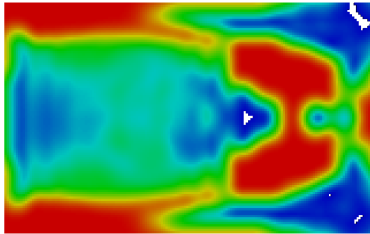
HDM Solution	HDM Gradient	ROB Construction	ROM Optimization
1049s (64)	88s (9)	727s (56)	39s (3676)

**CNQTR-MOR +  $\Phi_\mu$  adaptivity**

Elapsed time = 2197s, Speedup  $\approx 9x$



## Better Solution after 64 HDM Evaluations



HDM

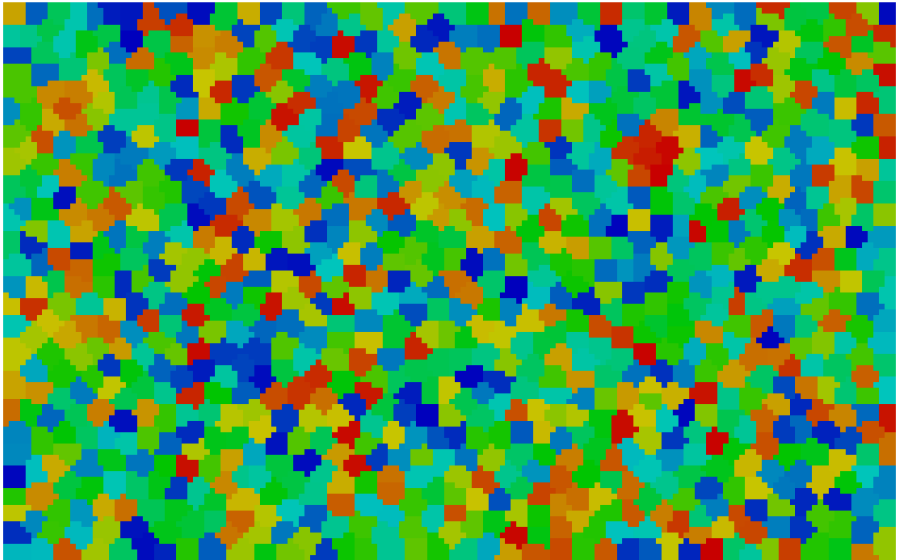


CNQTR-MOR +  $\Phi_\mu$  adaptivity

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



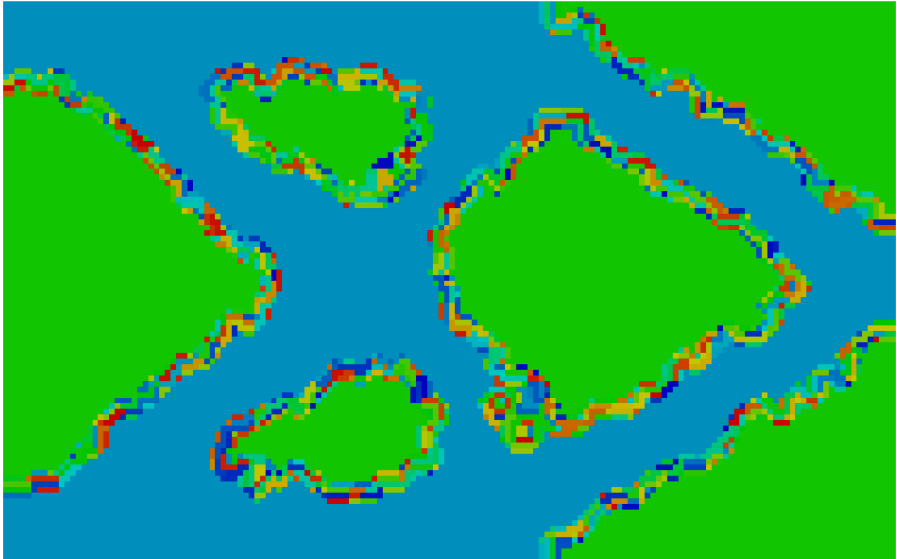
# Macro-element Evolution



Iteration 0 (1000)



# Macro-element Evolution



Iteration 1 (977)



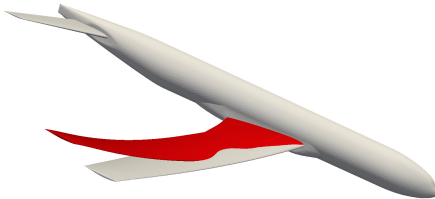
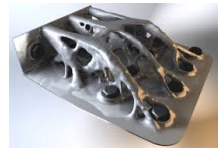
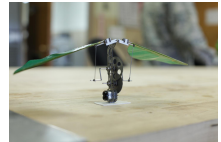
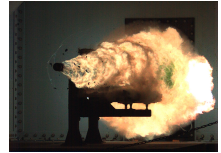
# CNQTR-MOR + $\Phi_\mu$ adaptivity



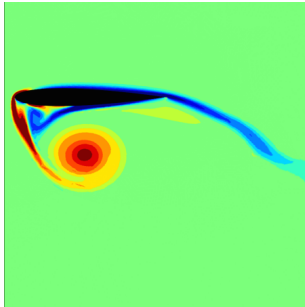


## Approaching Many-Query, Extreme-Scale Computational Physics

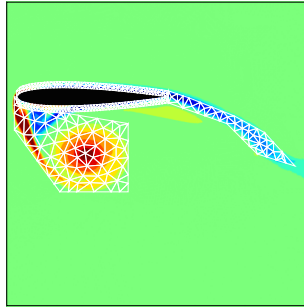
- Framework introduced for accelerating PDE-constrained optimization problem with **side constraints** and **large-dimensional parameter space**
- Speedup attained via adaptive reduction of state space and parameter space
- Concepts borrowed from constrained optimization theory
- Applied to aerodynamic design and topology optimization
  - Order of magnitude speedup observed
  - Competitive warm-start method



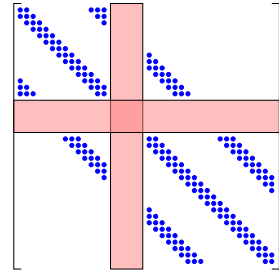
# Faster Computational Physics: Adaptive Data-Driven Discretization



(a) Vorticity around heaving airfoil



(b) Potential  $\Omega^l, \Omega^g$  decomposition



(c) Idealized sparsity structure

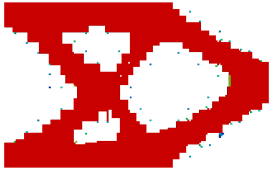
- Methods to *transform* features in global basis functions - minimize reliance on local shape functions
- Linear algebra for sparse operators with a few dense rows and columns
- Integration mesh to mitigate “variational crimes”



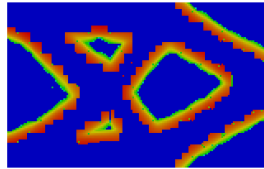
# Faster Solvers: Adaptive Reduction of High-Dimensional Optimization

$$\begin{aligned} & \underset{\mu}{\text{minimize}} && f(\mu) \\ & \text{subject to} && c(\mu) = 0 \end{aligned}$$

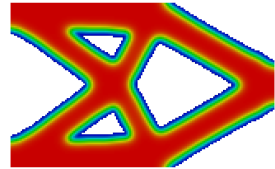
$$\begin{aligned} & \underset{y}{\text{minimize}} && f(\Phi_{\mu} \mu_{\tau}) \\ & \text{subject to} && c(\Phi_{\mu} \mu_{\tau}) = 0 \end{aligned}$$



(a) Sub-optimal sol'n



(b)  $|\nabla_{\mu} \mathcal{L}(\Phi_{\mu} \mu_{\tau}, \lambda)|$



(c) Optimal solution

- Prove global convergence and develop into general, constrained optimizer
- Further develop into topology optimization solver - *overcome checkerboarding*



## Fewer Queries: Second-Order Methods for Accelerated Convergence

Hessian information highly desired in optimization and UQ, but expensive due to  $\mathcal{O}(N_{\mu})$  required linear system solves

### Sensitivity/Adjoint Method for Computing Hessian

$$\frac{d^2 \mathcal{J}}{d\mu_j d\mu_k} = \frac{\partial^2 \mathcal{J}}{\partial \mu_j \partial \mu_k} + \frac{\partial^2 \mathcal{J}}{\partial \mu_j \partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mu_k} + \frac{\partial \mathbf{u}^T}{\partial \mu_j} \frac{\partial^2 \mathcal{J}}{\partial \mathbf{u} \partial \mu_k} + \frac{\partial \mathbf{u}^T}{\partial \mu_j} \frac{\partial^2 \mathcal{J}}{\partial \mathbf{u} \partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mu_k} - \frac{\partial \mathcal{J}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \left[ \frac{\partial^2 \mathbf{r}}{\partial \mu_j \partial \mu_k} + \frac{\partial^2 \mathbf{r}}{\partial \mu_j \partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mu_k} + \frac{\partial^2 \mathbf{r}}{\partial \mu_k \partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mu_j} + \frac{\partial^2 \mathbf{r}}{\partial \mathbf{u} \partial \mathbf{u}} : \frac{\partial \mathbf{u}}{\partial \mu_j} \otimes \frac{\partial \mathbf{u}}{\partial \mu_k} \right]$$

where

$$\frac{\partial \mathbf{u}}{\partial \mu_j} = \frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \mu_j}$$

- Fast, *multiple right-hand side* linear solver by building data-driven subspace for image of  $\frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}}$ ,  $\frac{\partial \mathbf{r}^{-T}}{\partial \mathbf{u}}$
- Similar to Krylov methods that use *a-priori, analytical* subspace



# Acknowledgement



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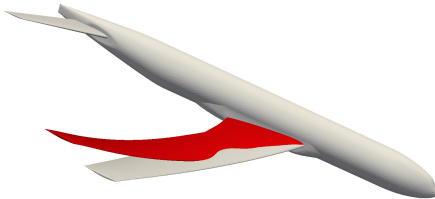
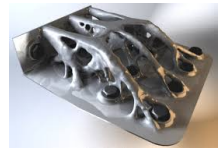
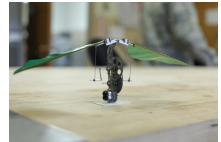
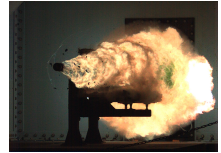
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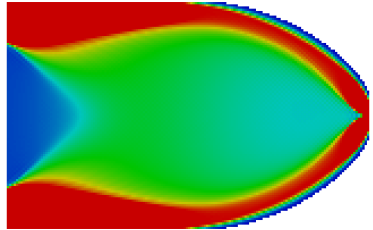


## Approaching Many-Query, Extreme-Scale Computational Physics

- 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 constrained optimization theory
- Applied to aerodynamic design and topology optimization
  - Order of magnitude speedup observed
  - Competitive warm-start method



# Standard Difficulty: Binary Solutions



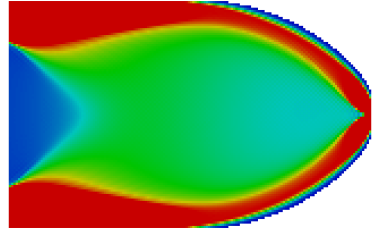
(a) Without penalization



# Standard Difficulty: Binary Solutions

## Relaxed, Penalized Problem Setup

$$\begin{aligned} & \text{minimize}_{\mathbf{u} \in \mathbb{R}^{n_u}, \boldsymbol{\mu} \in \mathbb{R}^{n_\mu}} && \mathbf{f}_{\text{ext}}^T \mathbf{u} \\ & \text{subject to} && V(\boldsymbol{\mu}) \leq \frac{1}{2} V_0 \\ & && \mathbf{r}(\mathbf{u}, \boldsymbol{\mu}^p) = 0 \\ & && \boldsymbol{\mu} \in [0, 1]^{k_\mu} \end{aligned}$$



(a) Without penalization

## Effect of Penalization

$$\mathbf{K}^e \leftarrow (\boldsymbol{\mu}^e)^p \mathbf{K}^e$$

- $\mathbf{K}^e$  : eth element stiffness matrix



# Standard Difficulty: Binary Solutions

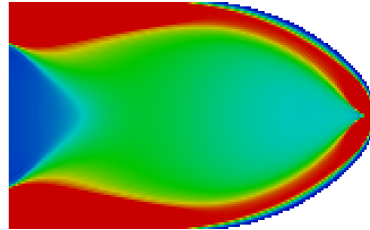
## Relaxed, Penalized Problem Setup

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

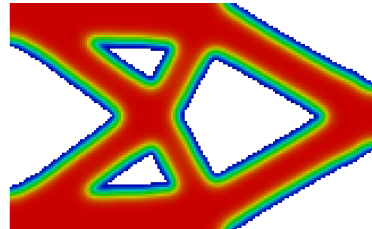
## Effect of Penalization

$$\mathbf{K}^e \leftarrow (\boldsymbol{\mu}^e)^p \mathbf{K}^e$$

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(a) Without penalization



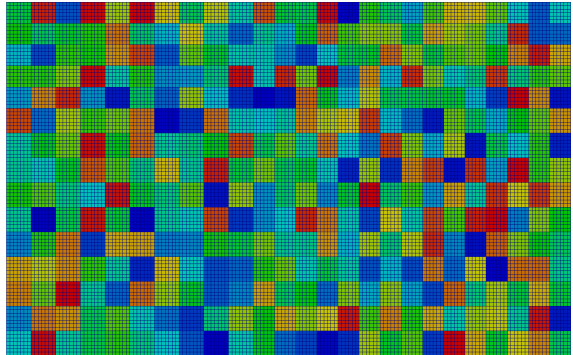
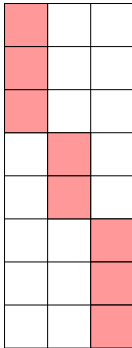
(b) With penalization



# Standard Difficulty: Binary Solutions

## Implication for ROM

- From parameter restriction,  $\boldsymbol{\mu}^p = (\Phi_{\boldsymbol{\mu}} \boldsymbol{\mu}_r)^p$
- Precomputation relies on separability of  $\Phi_{\boldsymbol{\mu}}$  and  $\boldsymbol{\mu}_r$
- Separability maintained if  $(\Phi_{\boldsymbol{\mu}} \boldsymbol{\mu}_r)^p = \Phi_{\boldsymbol{\mu}} \boldsymbol{\mu}_r^p$
- Sufficient condition: *columns of  $\Phi_{\boldsymbol{\mu}}$  have non-overlapping non-zeros*



## Efficient Evaluation of Nonlinear Terms

- Due to the mixing of high-dimensional and low-dimensional terms in the ROM expression, only limited speedups available

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

- To enable *pre-computation* of all large-dimensional quantities into low-dimensional ones, leverage *Taylor series expansion*

$$\begin{aligned} [\mathbf{r}_r(\mathbf{u}_r, \boldsymbol{\mu}_r)]_i &= \mathbf{D}_{im}^0(\boldsymbol{\mu}_r)_m + \mathbf{D}_{ijm}^1(\mathbf{u}_r \times \boldsymbol{\mu}_r)_{jm} + \mathbf{D}_{ijkm}^2(\mathbf{u}_r \times \mathbf{u}_r \times \boldsymbol{\mu}_r)_{jkm} \\ &\quad + \mathbf{D}_{ijklm}^3(\mathbf{u}_r \times \mathbf{u}_r \times \mathbf{u}_r \times \boldsymbol{\mu}_r)_{jklm} = 0 \end{aligned}$$

where

$$\mathbf{D}_{ijklm}^3 = \frac{\partial^3 \mathbf{r}_t}{\partial \mathbf{u}_p \partial \mathbf{u}_q \partial \mathbf{u}_s}(\hat{\mathbf{u}}, \boldsymbol{\phi}_{\boldsymbol{\mu}}^m)(\boldsymbol{\phi}_{\mathbf{u}}^i \times \boldsymbol{\phi}_{\mathbf{u}}^j \times \boldsymbol{\phi}_{\mathbf{u}}^k \times \boldsymbol{\phi}_{\mathbf{u}}^l)_{tpqs}$$

- Related work: [Rewienski, 2003, Barrault et al., 2004, Barbič and James, 2007, Nguyen and Peraire, 2008, Chaturantabut and Sorensen, 2010, Carlberg et al., 2011]



# Lagrange Multiplier Estimate

## Lagrange Multiplier, Constraint Pairs

$\lambda$	$\lambda_r$	$\tau$	$\tau_r$
$\mathbf{c}(\mathbf{u}, \boldsymbol{\mu}) \geq 0$	$\mathbf{c}(\Phi_{\mathbf{u}}\mathbf{u}_r, \Phi_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) \geq 0$	$\mathbf{A}\boldsymbol{\mu} \geq \mathbf{b}$	$\mathbf{A}_r\boldsymbol{\mu}_r \geq \mathbf{b}_r$

Goal: Given  $\mathbf{u}_r, \boldsymbol{\mu}_r, \boldsymbol{\tau}_r \geq 0, \boldsymbol{\lambda}_r \geq 0$ , estimate  $\tilde{\boldsymbol{\tau}} \geq 0, \tilde{\boldsymbol{\lambda}} \geq 0$  to compute

$$\nabla_{\boldsymbol{\mu}} \mathcal{L}(\Phi_{\boldsymbol{\mu}}\boldsymbol{\mu}_r, \tilde{\boldsymbol{\lambda}}, \tilde{\boldsymbol{\tau}}) = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\mu}}(\Phi_{\mathbf{u}}\mathbf{u}_r, \Phi_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) - \frac{\partial \mathbf{c}}{\partial \boldsymbol{\mu}}(\Phi_{\mathbf{u}}\mathbf{u}_r, \Phi_{\boldsymbol{\mu}}\boldsymbol{\mu}_r)^T \tilde{\boldsymbol{\lambda}} - \mathbf{A}^T \tilde{\boldsymbol{\tau}}$$

## Lagrange Multiplier Estimates

$$\tilde{\boldsymbol{\lambda}} = \boldsymbol{\lambda}_r$$

$$\tilde{\boldsymbol{\tau}} = \arg \min_{\boldsymbol{\tau} \geq 0} \left\| \mathbf{A}^T \boldsymbol{\tau} - \left( \frac{\partial \mathcal{J}}{\partial \boldsymbol{\mu}}(\Phi_{\mathbf{u}}\mathbf{u}_r, \Phi_{\boldsymbol{\mu}}\boldsymbol{\mu}_r) - \frac{\partial \mathbf{c}}{\partial \boldsymbol{\mu}}(\Phi_{\mathbf{u}}\mathbf{u}_r, \Phi_{\boldsymbol{\mu}}\boldsymbol{\mu}_r)^T \tilde{\boldsymbol{\lambda}} \right) \right\|$$

Non-negative least squares: [Lawson and Hanson, 1974, Chapman et al., 2015]



# Standard Difficulty: Checkerboarding

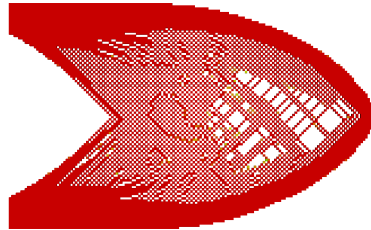
## Gradient Filtering, Nodal Projection

- Minimum length scale,  $r_{\min}$
- Gradient Filtering<sup>11</sup>

$$\frac{\widehat{\partial \mathcal{J}}}{\partial \boldsymbol{\mu}_k} = \frac{\sum_{j \in S_k} H_{kj} \boldsymbol{\mu}_i \frac{\partial \mathcal{J}}{\partial \boldsymbol{\mu}_i}}{\boldsymbol{\mu}_k \sum_{j \in S_k} H_{kj}}$$

- Nodal Projection

$$\boldsymbol{\mu}_k = \frac{\sum_{j \in S_k} \boldsymbol{\tau}_j H_{jk}}{\sum_{j \in S_k} H_{jk}}$$



(a) Without projection/filtering



<sup>11</sup> $H_{ki} = r_{\min} - \text{dist}(k, i)$



# Standard Difficulty: Checkerboarding

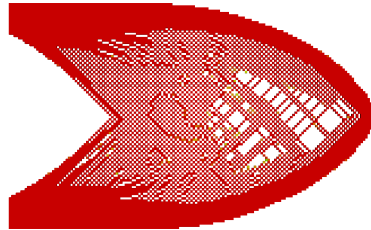
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- Minimum length scale,  $r_{\min}$
- Gradient Filtering<sup>11</sup>

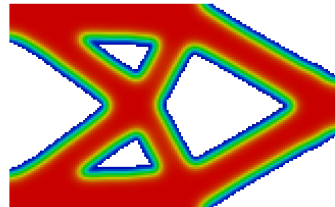
$$\frac{\widehat{\partial \mathcal{J}}}{\partial \boldsymbol{\mu}_k} = \frac{\sum_{j \in S_k} H_{kj} \boldsymbol{\mu}_i \frac{\partial \mathcal{J}}{\partial \boldsymbol{\mu}_i}}{\boldsymbol{\mu}_k \sum_{j \in S_k} H_{kj}}$$

- Nodal Projection

$$\boldsymbol{\mu}_k = \frac{\sum_{j \in S_k} \boldsymbol{\tau}_j H_{jk}}{\sum_{j \in S_k} H_{jk}}$$



(a) Without projection/filtering



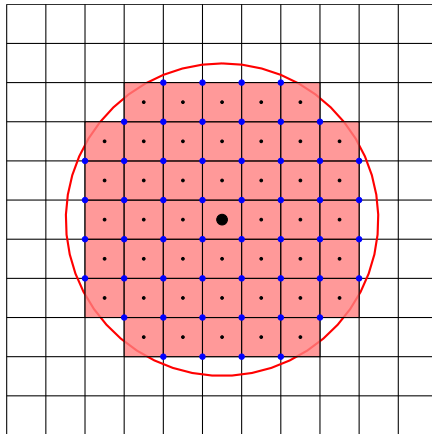
(b) With projection



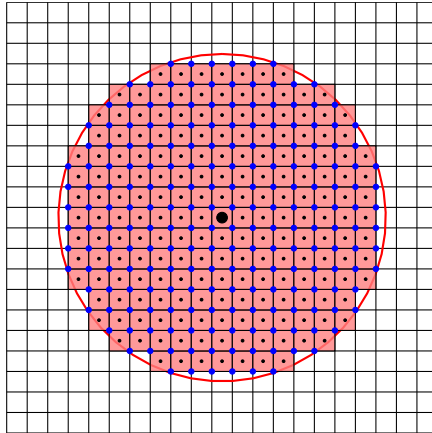
<sup>11</sup>  $H_{ki} = r_{\min} - \text{dist}(k, i)$



# Standard Difficulty: Checkerboarding



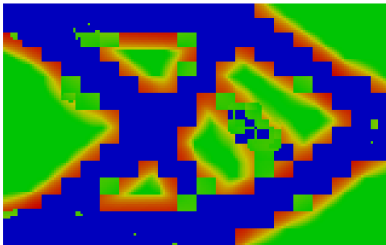
# Standard Difficulty: Checkerboarding



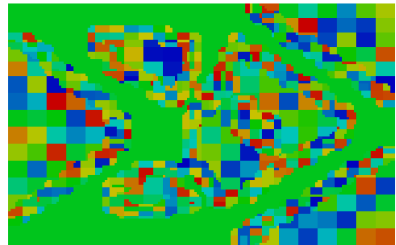
# Standard Difficulty: Checkerboarding

## Implication for ROM

- Nonlocality introduced through projection/filtering
- $\mu_e$  influences volume fraction of all elements within  $r_{\min}$  of element/node  $e$
- Clashes with requirement on  $\Phi_\mu$  of columns with non-overlapping non-zeros
- Handled heuristically by performing parameter basis adaptation to eliminate “checkerboard” regions of parameter space, uses concept of  $r_{\min}$
- *Next: Helmholtz filtering*



Gradient of Lagrangian



Updated Macroelements

