A Nonlinear Trust Region Framework for PDE-Constrained Optimization Using Progressively-Constructed Reduced-Order Models

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1. Motivation
2. PDE-Constrained Optimization
3. ROM-Constrained Optimization
4. Numerical Experiments
   - Airfoil Design
   - Rocket Nozzle Design
5. Conclusion

Reduced-Order Models (ROMs)

ROMs as Enabling Technology

- Many-query analyses
  - Optimization: design, control
    - Single objective, single-point
    - Multiobjective, multi-point
  - Uncertainty Quantification
    - Optimization under uncertainty
- Real-time analysis
  - Model Predictive Control (MPC)

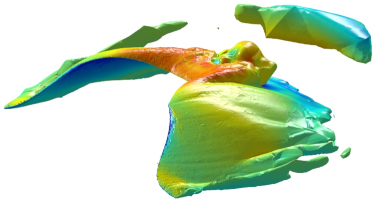
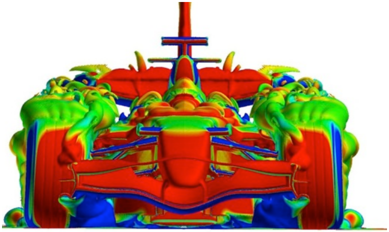
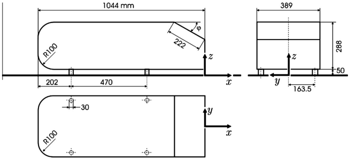


Figure: Flapping Wing (Persson et al., 2012)

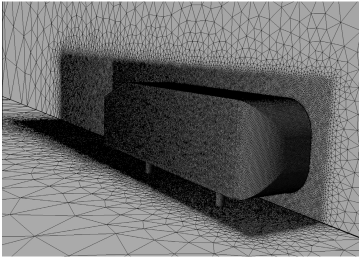


Application I: Compressible, Turbulent Flow over Vehicle

- Benchmark in automotive industry
- Mesh
  - 2,890,434 vertices
  - 17,017,090 tetra
  - 17,342,604 DOF
- CFD
  - Compressible Navier-Stokes
  - DES + Wall func
- Single forward simulation
  - $\approx$ 0.5 day on 512 cores
- Desired: shape optimization
  - unsteady effects
  - minimize average drag



(a) Ahmed Body: Geometry (Ahmed et al, 1984)



(b) Ahmed Body: Mesh (Carlberg et al, 2011)

Application II: Turbulent Flow over Flapping Wing

- Biologically-inspired flight
  - Micro aerial vehicles
- Mesh
  - 43,000 vertices
  - 231,000 tetra ($p = 3$)
  - 2,310,000 DOF
- CFD
  - Compressible Navier-Stokes
  - Discontinuous Galerkin
- Desired: shape optimization + control
  - unsteady effects
  - maximize thrust

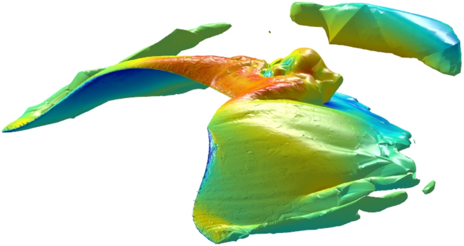


Figure: Flapping Wing (Persson et al., 2012)

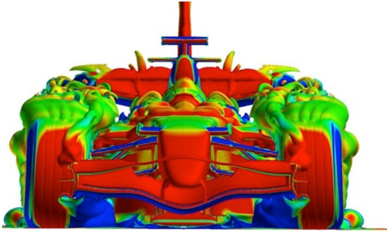
Problem Formulation

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

$$\begin{aligned} \underset{\mathbf{w}\in\mathbb{R}^N,\ \boldsymbol{\mu}\in\mathbb{R}^p}{\text{minimize}} \quad & f(\mathbf{w}, \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{R}(\mathbf{w}, \boldsymbol{\mu}) = 0 \end{aligned}$$

Discretize-then-optimize

where $\mathbf{R} : \mathbb{R}^N \times \mathbb{R}^p \to \mathbb{R}^N$ is the discretized (steady, nonlinear) PDE, $\mathbf{w}$ is the PDE state vector, $\boldsymbol{\mu}$ is the vector of parameters, and N is **assumed to be very large**.



Definition of $\boldsymbol{\Phi}$: Proper Orthogonal Decomposition

- MOR assumption

$$\mathbf{w} - \bar{\mathbf{w}} \approx \boldsymbol{\Phi}\mathbf{y} \qquad \Longrightarrow \qquad \frac{\partial \mathbf{w}}{\partial \boldsymbol{\mu}} \approx \boldsymbol{\Phi}\frac{\partial \mathbf{y}}{\partial \boldsymbol{\mu}}$$

State-Sensitivity[1] POD

- Collect state and sensitivity snapshots by sampling HDM

$$\mathbf{X} = \begin{bmatrix} \mathbf{w}(\boldsymbol{\mu}_1) - \bar{\mathbf{w}} & \mathbf{w}(\boldsymbol{\mu}_2) - \bar{\mathbf{w}} & \cdots & \mathbf{w}(\boldsymbol{\mu}_n) - \bar{\mathbf{w}} \end{bmatrix}$$
$$\mathbf{Y} = \begin{bmatrix} \frac{\partial \mathbf{w}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_1) & \frac{\partial \mathbf{w}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_2) & \cdots & \frac{\partial \mathbf{w}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_n) \end{bmatrix}$$

- Use Proper Orthogonal Decomposition to generate reduced bases from each *individually*

$$\boldsymbol{\Phi}_{\mathbf{X}} = \mathrm{POD}(\mathbf{X})$$
$$\boldsymbol{\Phi}_{\mathbf{Y}} = \mathrm{POD}(\mathbf{Y})$$

- Concatenate to get ROB

$$\boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\Phi}_{\mathbf{X}} & \boldsymbol{\Phi}_{\mathbf{Y}} \end{bmatrix}$$

[1] (Washabaugh and Farhat, 2013),(Zahr and Farhat, 2014)

ROM-Constrained Optimization

ROM-constrained optimization:

$$\begin{aligned} \underset{\mathbf{y}\in\mathbb{R}^n,\ \boldsymbol{\mu}\in\mathbb{R}^p}{\text{minimize}} \quad & f(\bar{\mathbf{w}} + \mathbf{\Phi}\mathbf{y}, \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{\Psi}^T\mathbf{R}(\bar{\mathbf{w}} + \mathbf{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0 \end{aligned}$$

where

$$\mathbf{R}_r(\mathbf{y}, \boldsymbol{\mu}) = \mathbf{\Psi}^T\mathbf{R}(\bar{\mathbf{w}} + \mathbf{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0$$

is the reduced-order model

Progressive/Adaptive Approach

Progressive Approach to ROM-Constrained Optimization

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

$$
\begin{aligned}
\underset{\mathbf{y}\in\mathbb{R}^n,\ \boldsymbol{\mu}\in\mathbb{R}^p}{\text{minimize}} \quad & f(\bar{\mathbf{w}} + \mathbf{\Phi}\mathbf{y}, \boldsymbol{\mu}) \\
\text{subject to} \quad & \mathbf{\Psi}^T\mathbf{R}(\bar{\mathbf{w}} + \mathbf{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0 \\
& \frac{1}{2}||\mathbf{R}(\bar{\mathbf{w}} + \mathbf{\Phi}\mathbf{y}, \boldsymbol{\mu})||_2^2 \leq \epsilon
\end{aligned}
$$

- Use solution of above problem to enrich training and repeat until convergence

(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)

Progressive Approach

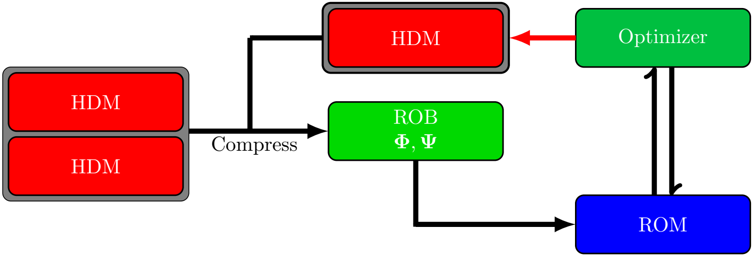
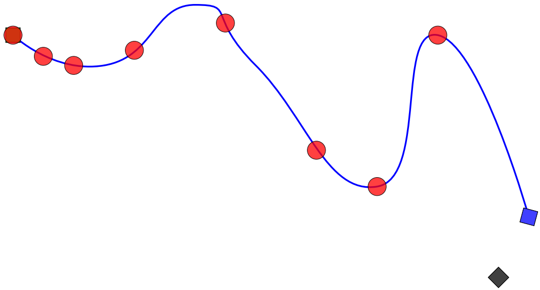
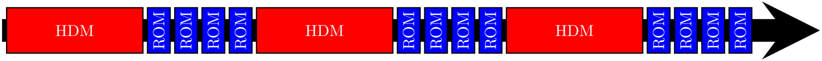


Figure: Schematic of Algorithm

Progressive Approach



(a) Idealized Optimization Trajectory: Parameter Space



(b) Breakdown of Computational Effort

Progressive Approach

Ingredients of Proposed Approach (Zahr and Farhat, 2014)

- Minimum-residual ROM (LSPG) and minimum-error sensitivities
  - $f_r(\boldsymbol{\mu}) = f(\boldsymbol{\mu}),\ \dfrac{\mathrm{d}f_r}{\mathrm{d}\boldsymbol{\mu}}(\boldsymbol{\mu}) = \dfrac{\mathrm{d}f}{\mathrm{d}\boldsymbol{\mu}}(\boldsymbol{\mu})$ for training parameters $\boldsymbol{\mu}$
- Reduced optimization (sub)problem

$$
\begin{aligned}
\underset{\mathbf{y}\in\mathbb{R}^n,\ \boldsymbol{\mu}\in\mathbb{R}^p}{\text{minimize}} \quad & f(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu}) \\
\text{subject to} \quad & \boldsymbol{\Psi}^T\mathbf{R}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu}) = 0 \\
& \frac{1}{2}||\mathbf{R}(\bar{\mathbf{w}} + \boldsymbol{\Phi}\mathbf{y}, \boldsymbol{\mu})||_2^2 \leq \epsilon
\end{aligned}
$$

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

Adaptive Selection of Trust-Region Radius

Let

$$\begin{aligned} \boldsymbol{\mu}_{-1}^* = \boldsymbol{\mu}_0^{(0)} &= \text{initial condition for PDE-constrained optimization} \\ \boldsymbol{\mu}_j^* &= \text{solution of } j\text{th reduced optimization problem} \end{aligned}$$

Define

$$\rho_j = \frac{f(\mathbf{w}(\boldsymbol{\mu}_j^*), \boldsymbol{\mu}_j^*) - f(\mathbf{w}(\boldsymbol{\mu}_{j-1}^*), \boldsymbol{\mu}_{j-1}^*)}{f(\mathbf{w}_r(\boldsymbol{\mu}_j^*), \boldsymbol{\mu}_j^*) - f(\mathbf{w}_r(\boldsymbol{\mu}_{j-1}^*), \boldsymbol{\mu}_{j-1}^*)}$$

Trust-Region Radius

$$\epsilon' = \begin{cases} \frac{1}{\tau}\epsilon & \rho_k \in [0.5, 2] \\ \epsilon & \rho_k \in [0.25, 0.5) \cup (2, 4] \\ \tau\epsilon & \text{otherwise} \end{cases}$$

Fast Updates to Reduced-Order Basis

Two situations where snapshot matrix modified (Zahr and Farhat, 2014)

- Additional snapshots to be incorporated

$$\mathbf{\Phi}' = \mathrm{POD}(\begin{bmatrix}\mathbf{X} & \mathbf{Y}\end{bmatrix}) \qquad \text{given} \qquad \mathbf{\Phi} = \mathrm{POD}(\mathbf{X})$$

- Offset vector modified

$$\mathbf{\Phi}' = \mathrm{POD}(\mathbf{X} - \tilde{\mathbf{w}}\mathbf{1}^T) \qquad \text{given} \qquad \mathbf{\Phi} = \mathrm{POD}(\mathbf{X} - \bar{\mathbf{w}}\mathbf{1}^T)$$

Compute new basis using singular factors of existing basis complete without complete recomputation

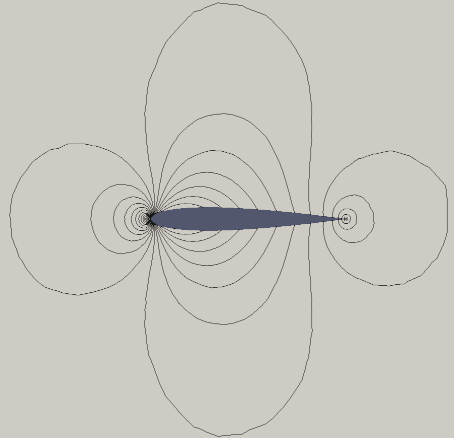
Fast, Low-Rank Updates to ROB

Compute (Brand, 2006)

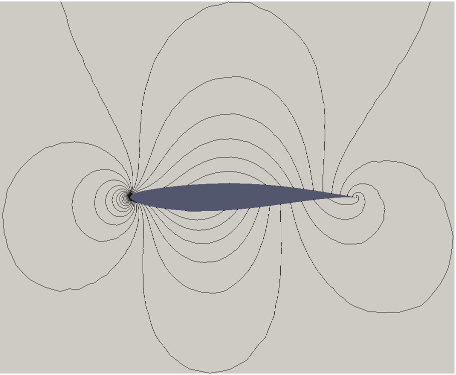
$$\mathbf{\Phi}' = \mathrm{POD}(\mathbf{X} + \mathbf{A}\mathbf{B}^T) \qquad \text{given} \qquad \mathbf{\Phi} = \mathrm{POD}(\mathbf{X})$$

- Large-scale SVD ($N \times n_{\text{snap}}$) replaced by small SVD (independent of N)
- Error incurred by using *truncated* basis $\propto \ \sigma_{n+1}$
  - Usually small in MOR applications

Compressible, Inviscid Airfoil Inverse Design



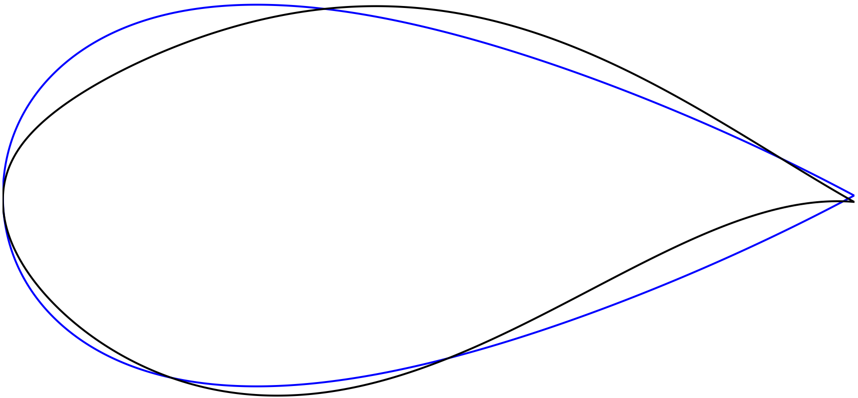
(a) NACA0012: Pressure field ($M_\infty = 0.5$, $\alpha = 0.0°$)



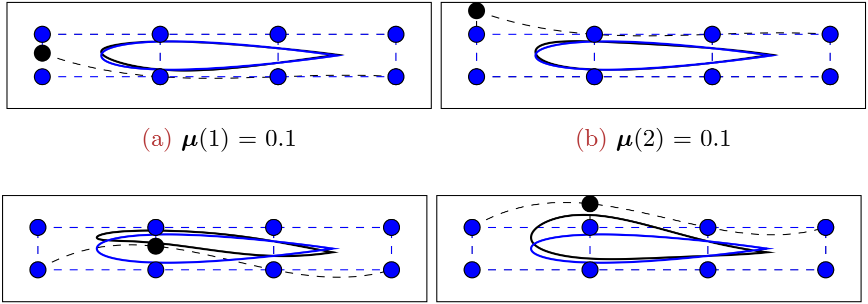
(b) RAE2822: Pressure field ($M_\infty = 0.5$, $\alpha = 0.0°$)

- Pressure discrepancy minimization (Euler equations)
  - Initial Configuration: NACA0012
  - Target Configuration: RAE2822

Initial/Target Airfoils: Scaled



Shape Parametrization

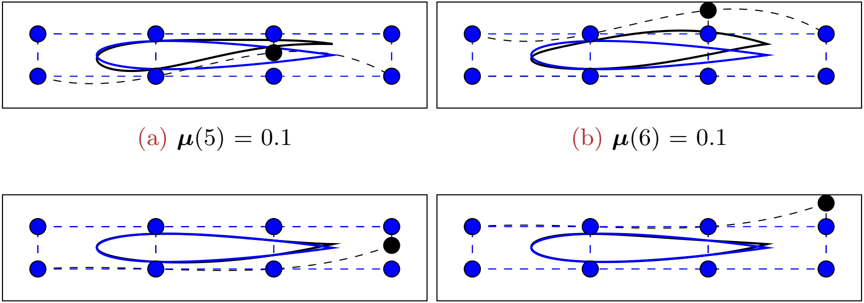


(a) $\boldsymbol{\mu}(1) = 0.1$ (b) $\boldsymbol{\mu}(2) = 0.1$

(c) $\boldsymbol{\mu}(3) = 0.1$ (d) $\boldsymbol{\mu}(4) = 0.1$

Figure: Shape parametrization of a NACA0012 airfoil using a *cubic* design element

Shape Parametrization

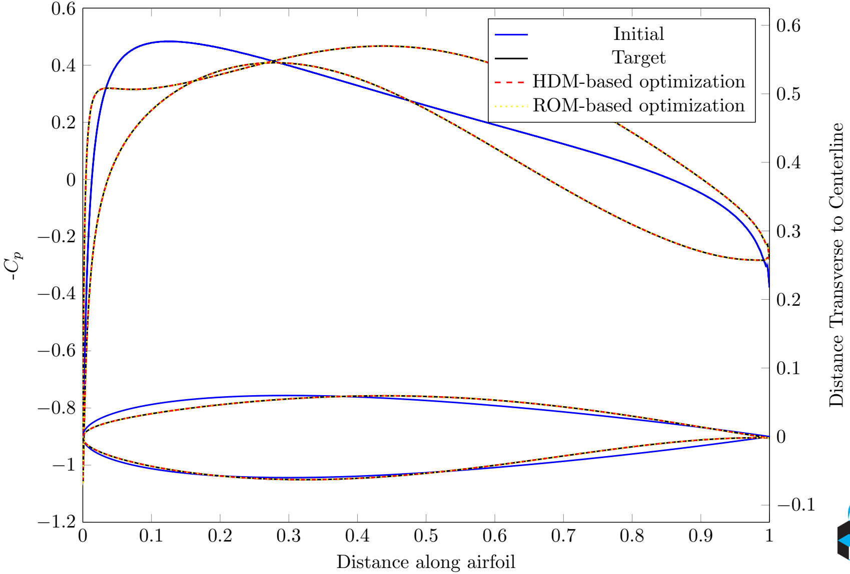


(a) $\boldsymbol{\mu}(5) = 0.1$ (b) $\boldsymbol{\mu}(6) = 0.1$

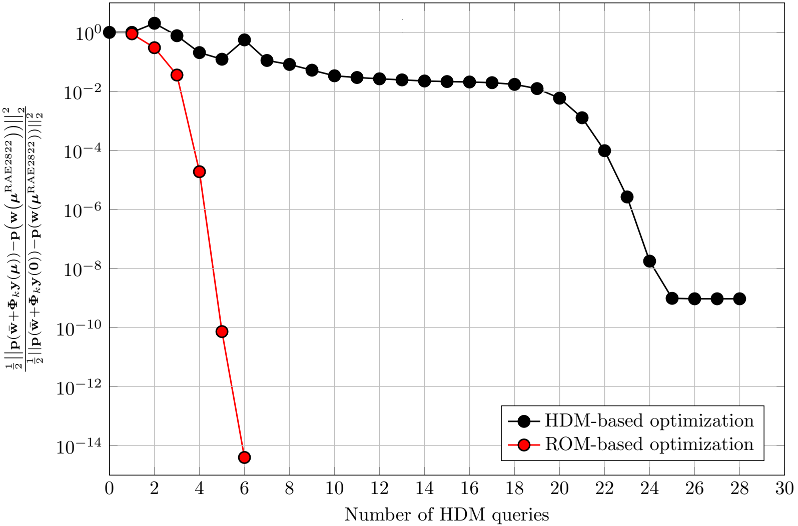
(c) $\boldsymbol{\mu}(7) = 0.1$ (d) $\boldsymbol{\mu}(8) = 0.1$

Figure: Shape parametrization of a NACA0012 airfoil using a *cubic* design element

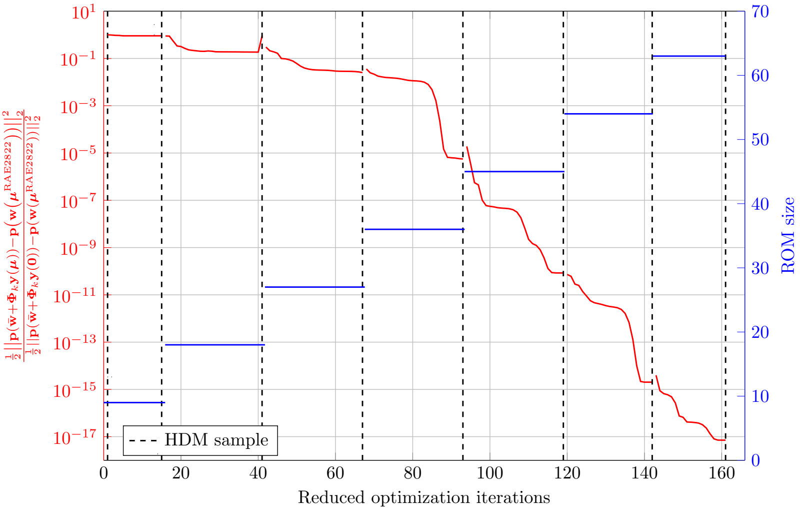
Optimization Results



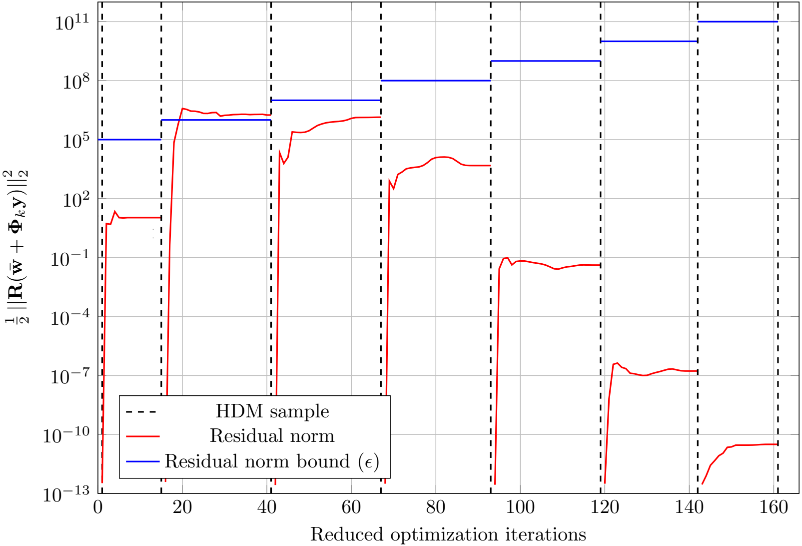
Optimization Results



Optimization Results



Optimization Results



Optimization Results

	HDM-based optimization	ROM-based optimization
# of HDM Evaluations	29	7
# of ROM Evaluations	-	346
$\dfrac{\|\|\boldsymbol{\mu}^* - \boldsymbol{\mu}^{RAE2822}\|\|}{\|\|\boldsymbol{\mu}^{RAE2822}\|\|}$	$2.28 \times 10^{-3}\%$	$4.17 \times 10^{-6}\%$

Table: Performance of the HDM- and ROM-based optimization methods

Quasi-1D Euler Flow

Quasi-1D Euler equations:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{1}{A}\frac{\partial (A\mathbf{F})}{\partial x} = \mathbf{Q}$$

where

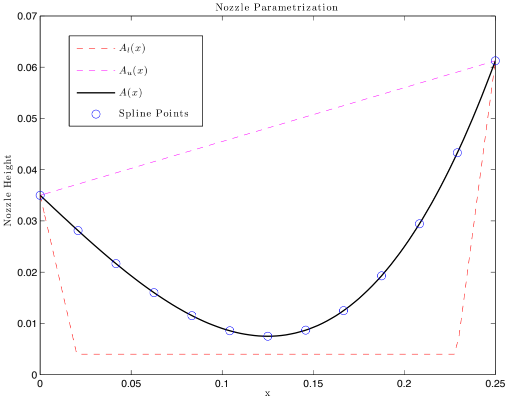
$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ e \end{bmatrix}, \qquad \mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (e+p)u \end{bmatrix}, \qquad \mathbf{Q} = \begin{bmatrix} 0 \\ \frac{p}{A}\frac{\partial A}{\partial x} \\ 0 \end{bmatrix}$$

- Semi-discretization
  - Finite Volume Method: constant reconstruction, 500 cells
  - Roe flux and entropy correction
- Full discretization
  - Backward Euler
  - Pseudo-transient integration to steady state

Nozzle Parametrization

Nozzle parametrized with *cubic splines* using 13 control points and constraints requiring

- convexity $A''(x) \geq 0$
- bounds on $A(x)$ $A_l(x) \leq A(x) \leq A_u(x)$
- bounds on $A'(x)$ at inlet/outlet $A'(x_l) \leq 0,\ A'(x_r) \geq 0$



Parameter Estimation/Inverse Design

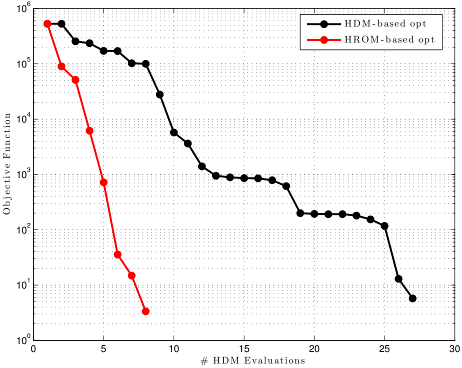
For this problem, the goal is to determine the parameter $\boldsymbol{\mu}^*$ such that the flow achieves some optimal or desired state $\mathbf{w}^*$

$$\begin{aligned} \underset{\mathbf{w}\in\mathbb{R}^N,\ \boldsymbol{\mu}\in\mathbb{R}^p}{\text{minimize}} \quad & ||\mathbf{w}(\boldsymbol{\mu}) - \mathbf{w}^*|| \\ \text{subject to} \quad & \mathbf{R}(\mathbf{w}, \boldsymbol{\mu}) = 0 \\ & \mathbf{c}(\mathbf{w}, \boldsymbol{\mu}) \leq 0 \end{aligned}$$

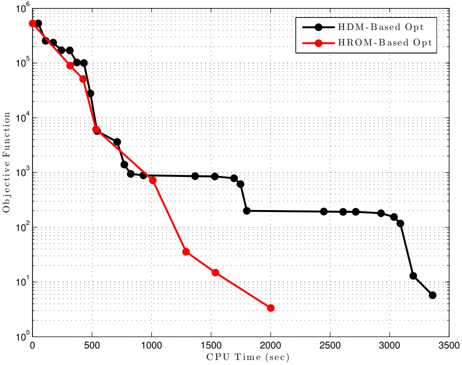
where $\mathbf{c}$ are the nozzle constraints.

Objective Function Convergence

(a) Convergence (# HDM Evals)

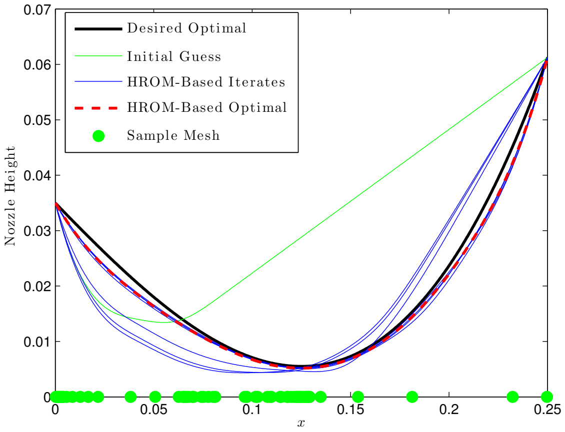


(b) Convergence (CPU Time)



Hyper-Reduced Optimization Progression

Figure: Parameter ($\boldsymbol{\mu}$) Progression



Optimization Summary

	HDM-Based Opt	HROM-Based Opt
Rel. Error in μ^* (%)	1.82	5.26
Rel. Error in w^* (%)	0.11	0.12
# HDM Evals	27	8
# HROM Evals	0	161
CPU Time (s)	3361.51	2001.74

Summary

Summary

- Introduced progressive, nonlinear trust region framework for reduced optimization
- Demonstrated approach on canonical problem from aerodynamic shape optimization
  - Factor of 4 fewer queries to HDM than standard PDE-constrained optimization approaches
- Preliminary results on toy problem regarding extension of framework to hyperreduction

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