Efficient PDE-Constrained Optimization using Adaptive Model Reduction

Matthew J. Zahr (mzahr@stanford.edu) and Charbel Farhat – Stanford University

Collaborators: Kevin Carlberg and Drew Kouri – Sandia National Laboratories

Motivation

Design and control of engineering systems driven by **high-fidelity computational models** have been become critical capabilities given the complexity of and **uncertainties** inherent in such systems. Optimization problems of this form may requires thousands of simulations, each of which may require millions of CPU-hours. We propose a **globally convergent** trust-region method for leveraging efficient **reduced-order models** to drastically reduce the cost of these optimization problems.

Deterministic Formulation

Goal: Efficiently solve **deterministic** PDE-constrained optimization problems

$$\underset{\boldsymbol{\mu}}{\text{minimize}} \quad \mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu}),\, \boldsymbol{\mu})$$

$\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{\mu})$ satisfies the discrete, **deterministic** PDE

$$\boldsymbol{r}(\boldsymbol{u};\, \boldsymbol{\mu}) = 0$$

$\boldsymbol{\mu}$ – optimization parameters

Stochastic Formulation

Goal: Efficiently solve **stochastic** PDE-constrained optimization problems

$$\underset{\boldsymbol{\mu}}{\text{minimize}} \quad \mathbb{E}[\mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu},\, \cdot),\, \boldsymbol{\mu},\, \cdot)]$$

$\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{\mu},\, \boldsymbol{\xi})$ satisfies the discrete, **stochastic** PDE

$$\boldsymbol{r}(\boldsymbol{u};\, \boldsymbol{\mu},\, \boldsymbol{\xi}) = 0 \quad \forall \boldsymbol{\xi} \in \Xi$$

$\boldsymbol{\mu}$ – optimization parameters, $\boldsymbol{\xi}$ – stochastic parameters

Error-Aware Trust-Region Model Management

Introduce a trust-region method to solve (1) that leverages *inexpensive* subproblems (2)

$$\underset{\boldsymbol{\mu}}{\text{minimize}} \quad F(\boldsymbol{\mu}) \qquad (1) \qquad\qquad \begin{array}{ll} \underset{\boldsymbol{\mu}}{\text{minimize}} & m_k(\boldsymbol{\mu}) \\ \text{subject to} & \vartheta_k(\boldsymbol{\mu}) \leq \Delta_k \end{array} \qquad (2)$$

where *there exists* a constant $\zeta > 0$ such that

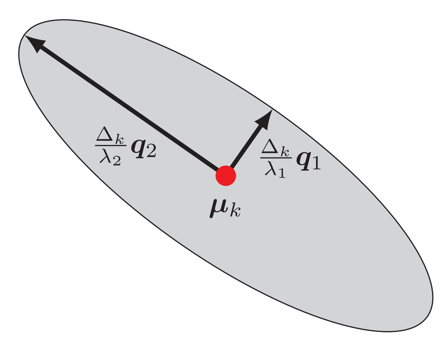
$$|F(\boldsymbol{\mu}) - m_k(\boldsymbol{\mu})| \leq \zeta \vartheta_k(\boldsymbol{\mu})$$

$$\boxed{\liminf_{k\to\infty} ||\nabla_{\boldsymbol{\mu}} F(\boldsymbol{\mu}_k)|| = 0}$$

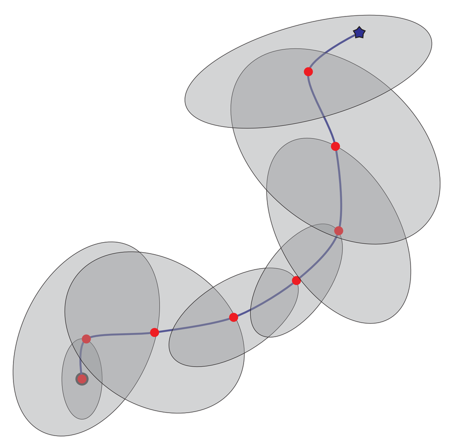
Error-aware TRs resemble traditional TRs in $\boldsymbol{\Theta}$-metric

$$\vartheta_k(\boldsymbol{\mu}) \equiv ||\boldsymbol{\vartheta}(\boldsymbol{\mu})|| \simeq ||\boldsymbol{\mu} - \boldsymbol{\mu}_k||_{\boldsymbol{\Theta}} \leq \Delta_k$$

$$\boldsymbol{\Theta} \equiv \partial_{\boldsymbol{\mu}} \boldsymbol{\vartheta}(\boldsymbol{\mu}_k)^T \partial_{\boldsymbol{\mu}} \boldsymbol{\vartheta}(\boldsymbol{\mu}_k) = \boldsymbol{Q}\boldsymbol{\Lambda}^2\boldsymbol{Q}^T$$



Error-aware trust region: $\boldsymbol{q}_i = \boldsymbol{Q}\boldsymbol{e}_i$, $\boldsymbol{\lambda}_i = \boldsymbol{e}_i\boldsymbol{\Lambda}\boldsymbol{e}_k$



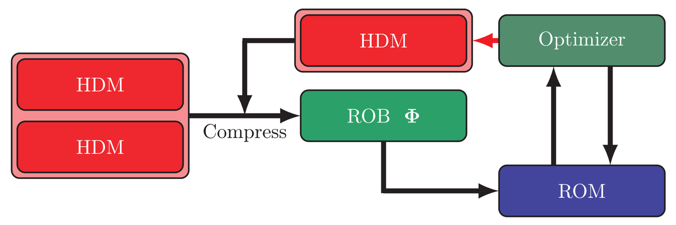
$\boldsymbol{\mu}$-space

Model Reduction

Model reduction *ansatz* and projection of governing equations

$$\boldsymbol{u} \approx \boldsymbol{\Phi}\boldsymbol{y} \qquad \Longrightarrow \qquad \boldsymbol{\Phi}^T\boldsymbol{r}(\boldsymbol{\Phi}\boldsymbol{y};\, \boldsymbol{\mu}) = 0$$

$\boldsymbol{\Phi}$ – *fixed*, *low*-dimenionsal subspace (very tall and skinny)



Trust-region model management framework

Deterministic Model Problem

ROM used to define inexpensive subproblem and residual used to manage inexactness

$$m_k(\boldsymbol{\mu}) \equiv \mathcal{J}(\boldsymbol{\Phi}_k\boldsymbol{y}(\boldsymbol{\mu}),\, \boldsymbol{\mu})$$
$$\vartheta_k(\boldsymbol{\mu}) \equiv ||\boldsymbol{r}(\boldsymbol{\Phi}_k\boldsymbol{y}(\boldsymbol{\mu});\, \boldsymbol{\mu})||$$

Stochastic Model Problem

Two-level inexactness – sparse grids to approximate integral and ROM to approximate function evaluations

$$m_k(\boldsymbol{\mu}) \equiv \mathbb{E}_{\mathcal{I}_k}\left[\mathcal{J}(\boldsymbol{\Phi}_k\boldsymbol{y}(\boldsymbol{\mu},\, \cdot),\, \boldsymbol{\mu},\, \cdot)\right]$$
$$\vartheta_k(\boldsymbol{\mu}) \equiv \mathbb{E}_{\mathcal{I}_k\cup\mathcal{N}(\mathcal{I}_k)}\left[||\boldsymbol{r}(\boldsymbol{\Phi}_k\boldsymbol{y}(\boldsymbol{\mu},\, \cdot);\, \boldsymbol{\mu})||\right] + \left|\mathbb{E}_{\mathcal{N}(\mathcal{I}_k)}\left[\mathcal{J}(\boldsymbol{\Phi}_k\boldsymbol{y}(\boldsymbol{\mu},\, \cdot),\, \boldsymbol{\mu},\, \cdot)\right]\right|$$

$\mathcal{I}_k$ – sparse grid $\qquad \mathcal{N}(\mathcal{I}_k)$ – neighbors of sparse grid

Risk-Neutral Optimal Control of Steady Burgers' Equation

Optimal control of stochastic Burgers' equation

$$\underset{\boldsymbol{\mu}}{\text{minimize}} \quad \int_{-1}^{1} \frac{1}{8}\left[\int_0^1 \frac{1}{2}(u-1)^2\, dx + \frac{\alpha}{2}\int_0^1 z(\boldsymbol{\mu},\, x)^2\, dx\right] d\boldsymbol{\xi}$$

$$-10^{\xi_1 - 2}\partial_{xx}u + u\partial_x u = z(\boldsymbol{\mu},\, x)$$

$$u(\boldsymbol{\mu},\, \boldsymbol{\xi},\, 0) = 1 + \frac{\xi_2}{1000} \qquad u(\boldsymbol{\mu},\, \boldsymbol{\xi},\, 1) = \frac{\xi_3}{1000}$$

$z(\boldsymbol{\mu},\, x)$ – parametrized by 9 cubic splines (11 parameters)

	HDM Queries	ROM Queries (max size)
HDM opt	6372	-
ROM opt	4	3720 (48)

Comparison of ROM optimization with error-aware trust-region model management to HDM optimization on 4-level isotropic sparse grid

$m_k(\boldsymbol{\mu}_k)$	$F(\boldsymbol{\mu}_k)$	$\|\|\nabla F(\boldsymbol{\mu}_k)\|\|$	Δ_k	Success?
3.8783e-03	8.3351e-03	6.8542e-03	-	-
3.1121e-03	7.2687e-03	7.0676e-03	1.0000e+02	True
3.0474e-03	6.8352e-03	3.3518e-03	2.0000e+02	True
1.1910e-02	9.7269e-03	3.5655e-03	1.0000e+02	False
6.3680e-03	6.3591e-03	8.6182e-05	2.8202e-03	True
6.3587e-03	6.3589e-03	7.2665e-07	5.6404e-03	True

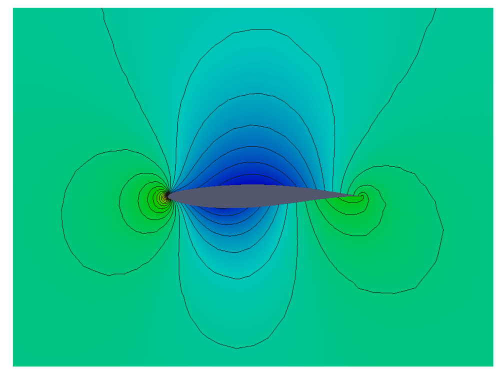
Convergence history of error-aware trust-region method

Inviscid, Subsonic Aerodynamic Shape Design

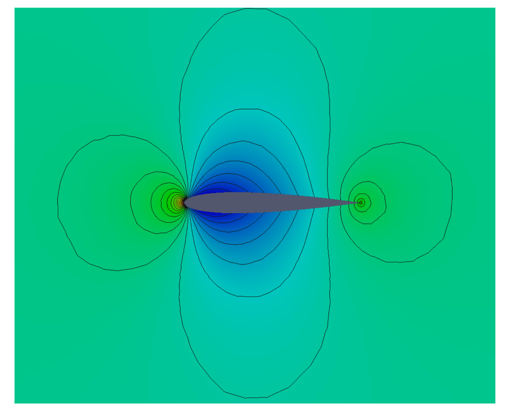
Inviscid inverse shape design

$$\underset{\boldsymbol{\mu}}{\text{minimize}} \quad ||\boldsymbol{p}(\boldsymbol{\mu}) - \boldsymbol{p}^*||$$

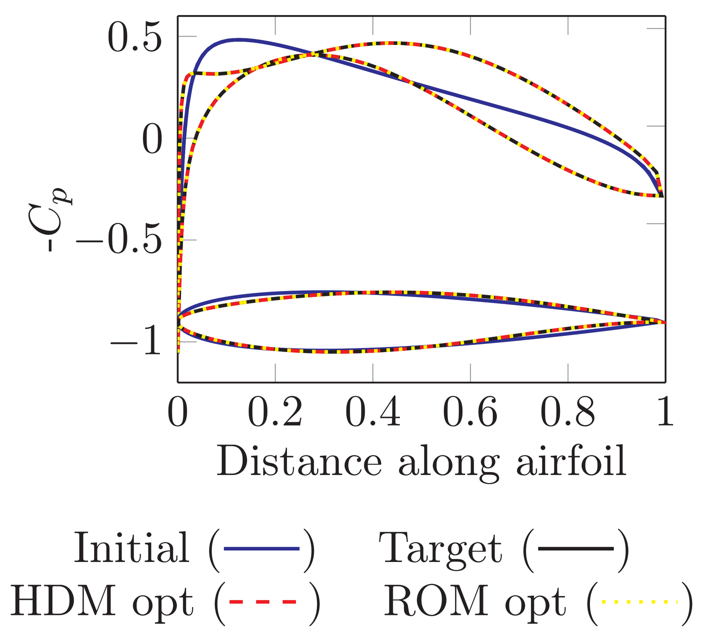
$\boldsymbol{p}(\boldsymbol{\mu})$ – pressure distribution around $\boldsymbol{\mu}$-foil
$\boldsymbol{p}^*$ – pressure distribution around RAE2822

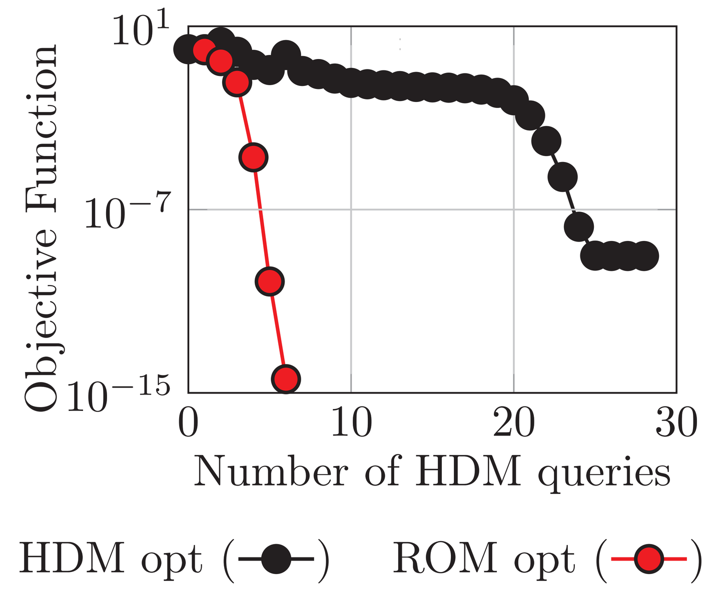


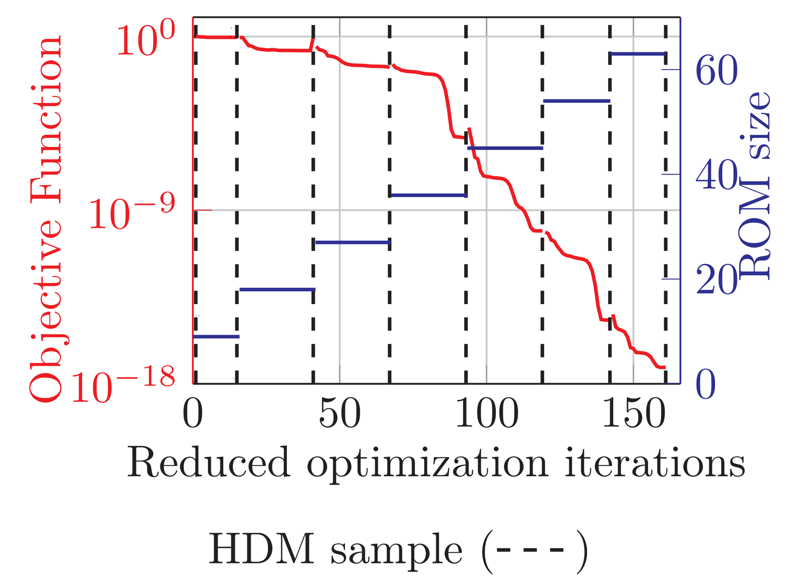
Initial Shape (NACA0012)



Target Shape (RAE2822)





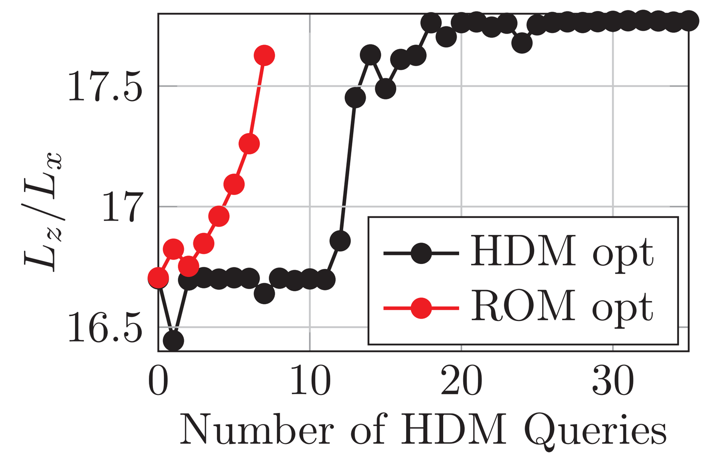


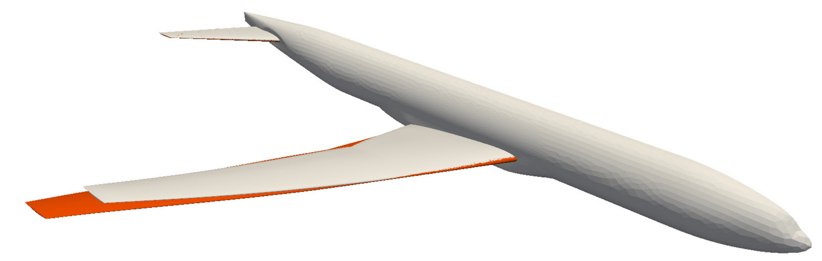
Turbulent, Transonic Aerodynamic Shape Design of Full Aircraft

Turbulent, transconic shape design

$$\underset{\boldsymbol{\mu}}{\text{maximize}} \quad L_z(\boldsymbol{\mu})/L_x(\boldsymbol{\mu})$$

$L_x(\boldsymbol{\mu})$, $L_z(\boldsymbol{\mu})$ – drag, lift at shape $\boldsymbol{\mu}$





Initial (gray) and optimal (red) shape

Conclusions

Leveraging and managing inexactness for efficient deterministic and stochastic PDE-constrained optimization

This work introduced a framework for leveraging reduced-order models and adaptive, anisotropic sparse grids to efficiently solve PDE-constrained optimization problems **ensuring convergence to a critical point of the original problem**. By breaking the offline-online decomposition commonly employed in model reduction, sampling and integration in high-dimensional spaces is avoided. The method is demonstrated on series of computational mechanics problems, including a large-scale industrial example.