Adaptive model reduction to accelerate optimization problems governed by partial differential equations

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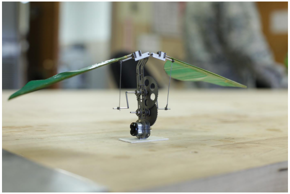
PDE optimization is ubiquitous in science and engineering

Design: Find system that optimizes performance metric, satisfies constraints

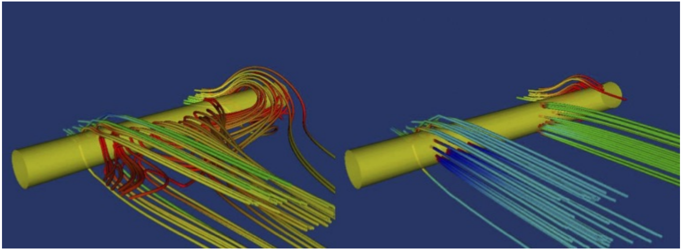
Aerodynamic shape design of automobile



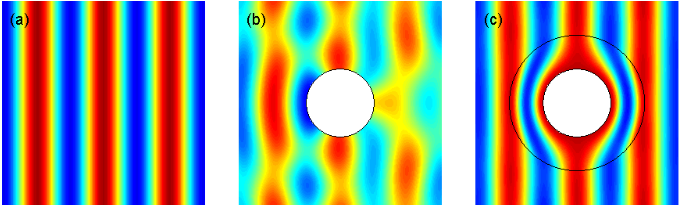
Optimal flapping motion of micro aerial vehicle

PDE optimization is ubiquitous in science and engineering

Control: Drive system to a desired state



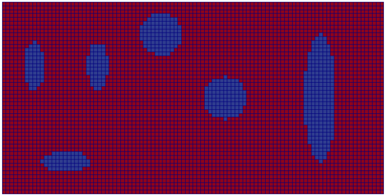
Boundary flow control

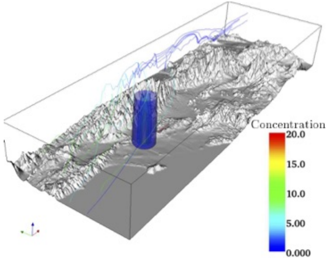


Metamaterial cloaking – electromagnetic invisibility

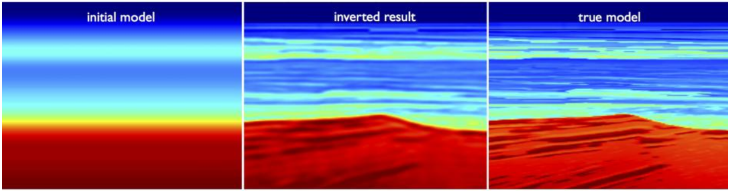
PDE optimization is ubiquitous in science and engineering

Inverse problems: Infer the problem setup given solution observations





Left: Material inversion – find inclusions from acoustic, structural measurements
Right: Source inversion – find source of airborne contaminant from downstream measurements

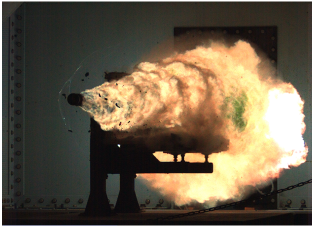


Full waveform inversion – estimate subsurface of Earth's crust from acoustic

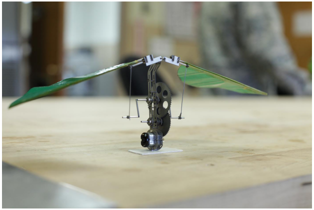
PDE optimization – a key player in next-gen problems

*Current interest in **computational physics** reaches far beyond analysis of a single configuration of a physical system into **design** (shape and topology) and **control** in an **uncertain** setting*

Engine System



EM Launcher



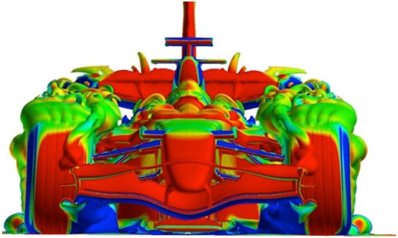
Micro-Aerial Vehicle

Repeated queries to **high-fidelity simulations** required by optimization and uncertainty quantification may be **prohibitively time-consuming**

Deterministic PDE-constrained optimization formulation

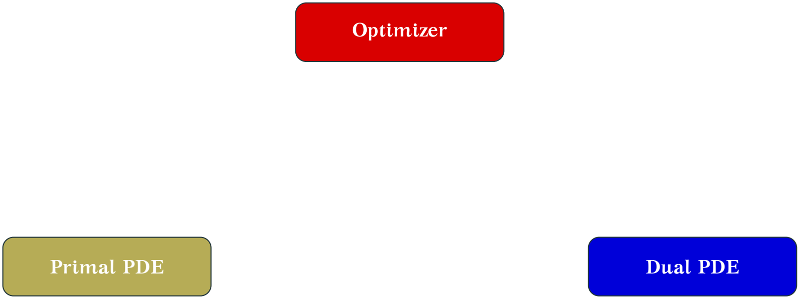
$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad \mathcal{J}(\mathbf{u}, \boldsymbol{\mu})$$
$$\text{subject to} \quad \mathbf{r}(\mathbf{u}; \boldsymbol{\mu}) = 0$$

- $\mathbf{r} : \mathbb{R}^{n_\mathbf{u}} \times \mathbb{R}^{n_\mu} \to \mathbb{R}^{n_\mathbf{u}}$ — discretized PDE
- $\mathcal{J} : \mathbb{R}^{n_\mathbf{u}} \times \mathbb{R}^{n_\mu} \to \mathbb{R}$ — quantity of interest
- $\mathbf{u} \in \mathbb{R}^{n_\mathbf{u}}$ — PDE state vector
- $\boldsymbol{\mu} \in \mathbb{R}^{n_\mu}$ — optimization parameters



Nested approach to PDE-constrained optimization

Virtually all expense emanates from primal/dual PDE solves



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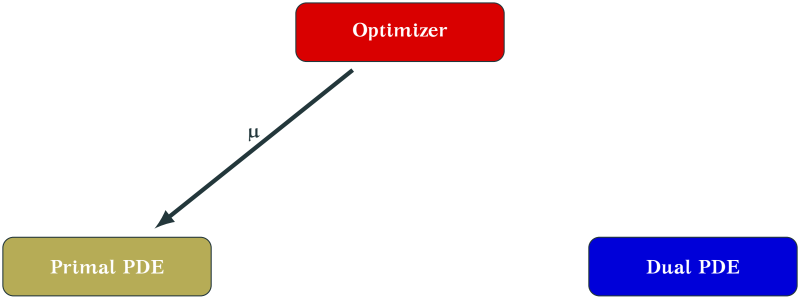

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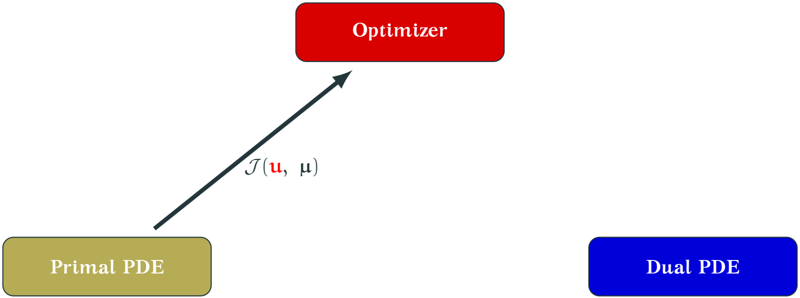

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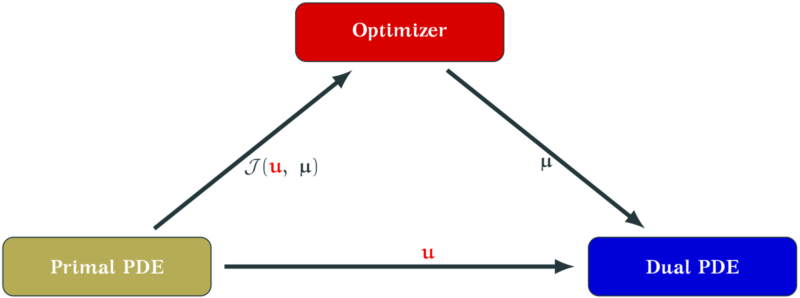

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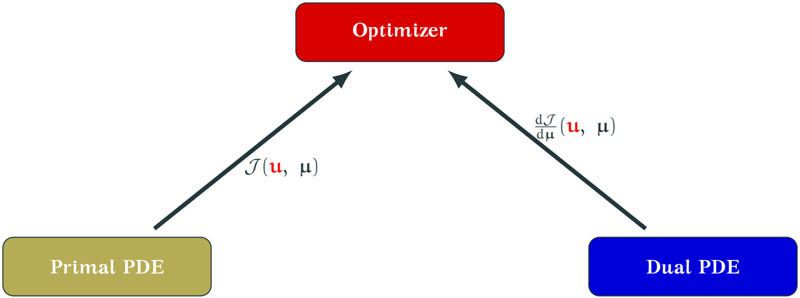


Application in computational mechanics: dynamic

Energy = 9.4096e+00 Thrust = 1.7660e-01	Energy = 4.9476e+00 Thrust = 2.5000e+00	Energy = 4.6110e+00 Thrust = 2.5000e+00
Initial	Optimal Control	Optimal Shape/Control

[Zahr and Persson, 2016], [Zahr et al., 2016c]

Stochastic PDE-constrained optimization formulation

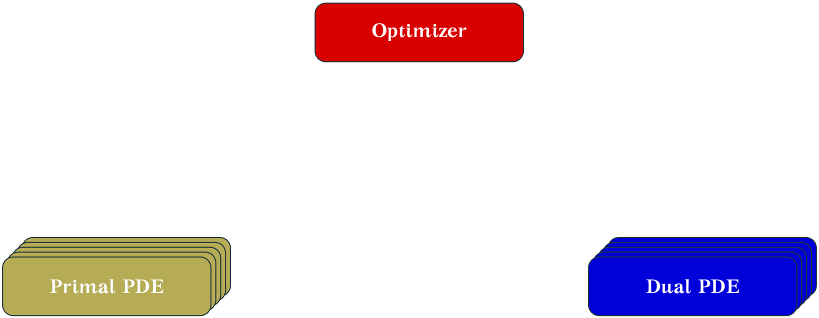
$$\begin{aligned} \underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad & \mathbb{E}[\mathcal{J}(\mathbf{u}, \boldsymbol{\mu}, \cdot)] \\ \text{subject to} \quad & \mathbf{r}(\mathbf{u}; \boldsymbol{\mu}, \boldsymbol{\xi}) = 0 \quad \forall \boldsymbol{\xi} \in \boldsymbol{\Xi} \end{aligned}$$

- $\mathbf{r} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \times \mathbb{R}^{n_\xi} \to \mathbb{R}^{n_u}$ — discretized stochastic PDE
- $\mathcal{J} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \times \mathbb{R}^{n_\xi} \to \mathbb{R}$ — quantity of interest
- $\mathbf{u} \in \mathbb{R}^{n_u}$ — PDE state vector
- $\boldsymbol{\mu} \in \mathbb{R}^{n_\mu}$ — (deterministic) optimization parameters
- $\boldsymbol{\xi} \in \mathbb{R}^{n_\xi}$ — stochastic parameters
- $\mathbb{E}[\mathcal{F}] \equiv \int_{\boldsymbol{\Xi}} \mathcal{F}(\boldsymbol{\xi})\rho(\boldsymbol{\xi})\, d\boldsymbol{\xi}$

*Each function evaluation requires integration over stochastic space – **expensive***

Nested approach to stochastic PDE-constrained optimization

Ensemble *of primal/dual PDE solves increases cost by* ***orders of magnitude***



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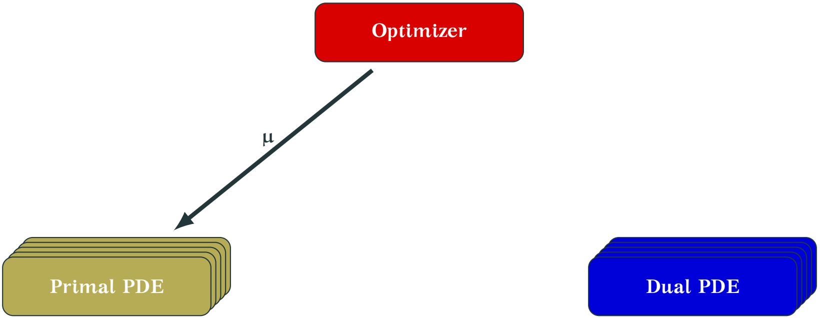

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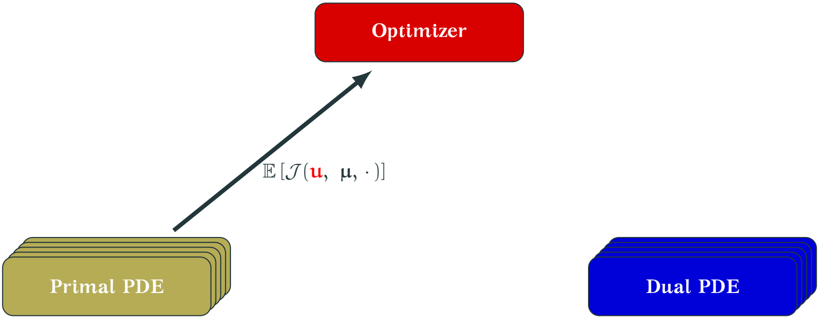

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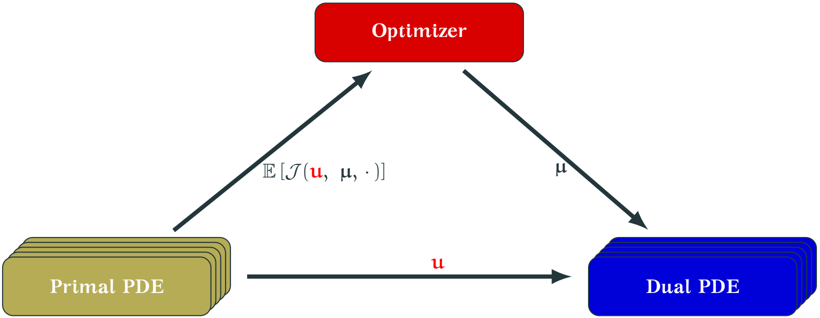

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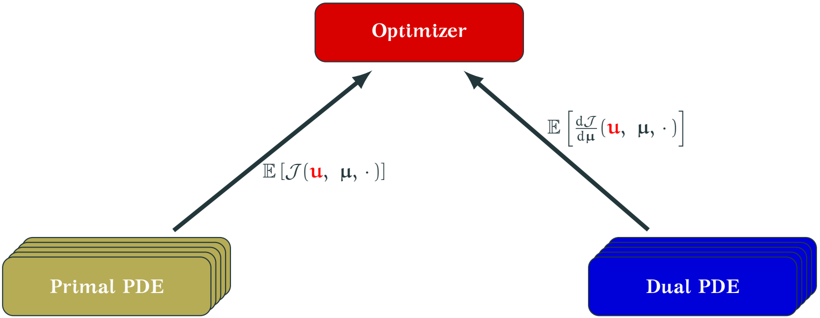

Proposed approach: managed inexactness

Replace expensive PDE with inexpensive approximation model

- **Reduced-order models** used for *inexact PDE evaluations*
- **Partially converged solutions** used for *inexact PDE evaluations*
- **Anisotropic sparse grids** used for *inexact integration* of risk measures

$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad F(\mu) \qquad \longrightarrow \qquad \underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad m_k(\mu)$$

Must be *computable* and apply to general, nonlinear PDEs

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Manage inexactness with trust region method

- Embedded in globally convergent **trust region** method
- **Error indicators**[1] to account for *all* sources of inexactness
- **Refinement** of approximation model using *greedy algorithms*

$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad F(\mu) \qquad \longrightarrow \qquad \begin{aligned} &\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} && m_k(\mu) \\ &\text{subject to} && \|\mu - \mu_k\| \leq \Delta_k \end{aligned}$$

[1] Must be *computable* and apply to general, nonlinear PDEs

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Relationship between the objective function and model

Asymptotic gradient bound permits the use of an ***error indicator****:* φ_k

$$\|\nabla F(\mu) - \nabla m_k(\mu)\| \leq \xi \varphi_k(\mu) \qquad \xi > 0$$

$$\varphi_k(\mu_k) \leq \kappa_\varphi \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$$

Trust region method with inexact gradients [Kouri et al., 2013]

1: **Model update**: Choose model m_k and error indicator φ_k

$$\varphi_k(\mu_k) \le \kappa_\varphi \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$$

2: **Step computation**: Approximately solve the trust region subproblem

$$\hat{\mu}_k = \underset{\mu \in \mathbb{R}^{n_\mu}}{\arg\min}\; m_k(\mu) \quad \text{subject to} \quad \|\mu - \mu_k\| \le \Delta_k$$

3: **Step acceptance**: Compute actual-to-predicted reduction

$$\rho_k = \frac{F(\mu_k) - F(\hat{\mu}_k)}{m_k(\mu_k) - m_k(\hat{\mu}_k)}$$

if $\rho_k \ge \eta_1$ **then** $\mu_{k+1} = \hat{\mu}_k$ **else** $\mu_{k+1} = \mu_k$ **end if**

4: **Trust region update**:

if $\rho_k \le \eta_1$ **then** $\Delta_{k+1} \in (0, \gamma \|\hat{\mu}_k - \mu_k\|]$ **end if**

if $\rho_k \in (\eta_1, \eta_2)$ **then** $\Delta_{k+1} \in [\gamma \|\hat{\mu}_k - \mu_k\|, \Delta_k]$ **end if**

if $\rho_k \ge \eta_2$ **then** $\Delta_{k+1} \in [\Delta_k, \Delta_{max}]$ **end if**

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Trust region method with inexact gradients and objective

1: **Model update**: Choose model m_k and error indicator φ_k

$$\vartheta_k(\mu_k) \leq \kappa_\vartheta \Delta_k \qquad \varphi_k(\mu_k) \leq \kappa_\varphi \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$$

2: **Step computation**: Approximately solve the trust region subproblem

$$\hat{\mu}_k = \underset{\mu \in \mathbb{R}^{n_\mu}}{\arg\min}\; m_k(\mu) \quad \text{subject to} \quad \vartheta_k(\mu) \leq \Delta_k$$

3: **Step acceptance**: Compute approximation of actual-to-predicted reduction

$$\rho_k = \frac{\psi_k(\mu_k) - \psi_k(\hat{\mu}_k)}{m_k(\mu_k) - m_k(\hat{\mu}_k)}$$

if $\rho_k \geq \eta_1$ **then** $\mu_{k+1} = \hat{\mu}_k$ **else** $\mu_{k+1} = \mu_k$ **end if**

4: **Trust region update**:

if $\rho_k \leq \eta_1$ **then** $\Delta_{k+1} \in (0, \gamma\vartheta_k(\hat{\mu}_k)]$ **end if**

if $\rho_k \in (\eta_1, \eta_2)$ **then** $\Delta_{k+1} \in [\gamma\vartheta_k(\hat{\mu}_k), \Delta_k]$ **end if**

if $\rho_k \geq \eta_2$ **then** $\Delta_{k+1} \in [\Delta_k, \Delta_{max}]$ **end if**

Inexact objective evaluations with asymptotic error bounds

Asymptotic accuracy requirements on approximation model [Zahr et al., 2016b]

$$|F(\mu_k) - F(\mu) + m_k(\mu) - m_k(\mu_k)| \leq \zeta \vartheta_k(\mu) \qquad \zeta > 0$$

$$\vartheta_k(\mu_k) \leq \kappa_\vartheta \Delta_k \qquad \kappa_\vartheta \in (0, 1)$$

Asymptotic accuracy requirements on inexact objective evaluations [Kouri et al., 2014]

$$|F(\mu_k) - F(\mu) + \psi_k(\mu) - \psi_k(\mu_k)| \leq \sigma \theta_k(\mu) \qquad \sigma > 0$$

$$\theta_k(\hat{\mu}_k)^\omega \leq \eta \min\{m_k(\mu_k) - m_k(\hat{\mu}_k), r_k\}$$

$$\omega, \eta \in (0, 1), \; r_k \rightarrow 0$$

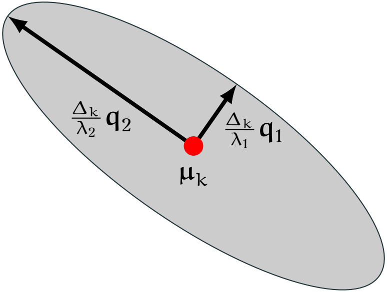
An interpretation of error-aware trust regions

Let $\boldsymbol{\vartheta}_k(\boldsymbol{\mu})$ be a vector-valued error indicator such that $\vartheta_k(\boldsymbol{\mu}) = \|\boldsymbol{\vartheta}_k(\boldsymbol{\mu})\|_2$ and

$$\mathbf{A}_k = \frac{\partial \boldsymbol{\vartheta}_k}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_k)^T \frac{\partial \boldsymbol{\vartheta}_k}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_k) = \mathbf{Q}_k \boldsymbol{\Lambda}_k^2 \mathbf{Q}_k^T$$

Then, to first order[2],

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



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

[2] assuming $\vartheta_k(\boldsymbol{\mu}_k) = 0$, i.e., model exact at trust region center

A look at error-aware trust regions

Optimization of the Rosenbrock function

$$\underset{\mu \in \mathbb{R}^2}{\text{minimize}} \quad F(\mu) \equiv 100(\mu_2 - \mu_1^2)^2 + (1 - \mu_1)^2.$$

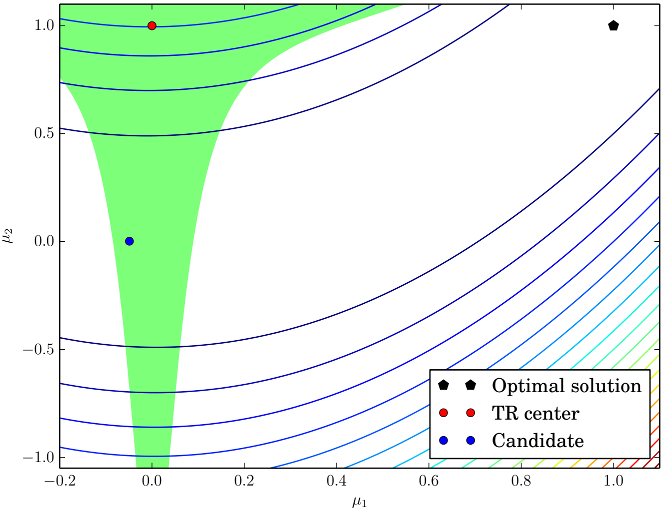
using the approximation models and error indicators

$$\begin{aligned} m_k(\mu) &\equiv G_k(\mu;\ \epsilon_k,\ \delta_k) \\ \psi_k(\mu) &\equiv F(\mu) \\ \vartheta_k(\mu) &\equiv |F(\mu) - G_k(\mu;\ \epsilon_k,\ \delta_k)| + |F(\mu_k) - G_k(\mu_k;\ \epsilon_k,\ \delta_k)| \\ \varphi_k(\mu) &\equiv \|\nabla F(\mu) - \nabla G_k(\mu;\ \epsilon_k,\ \delta_k)\| \\ \theta_k(\mu) &\equiv 0 \end{aligned}$$

where $G_k(\mu;\ \epsilon_k,\ \delta_k)$ is the inexact quadratic approximation of F at μ_k

$$G_k(\mu;\ \epsilon,\ \delta) \equiv F(\mu_k) + \epsilon + (\nabla F(\mu_k) + \delta \mathbf{1})^T(\mu - \mu_k) + \frac{1}{2}(\mu - \mu_k)^T \nabla^2 F(\mu_k)(\mu - \mu_k)$$

A look at error-aware trust regions



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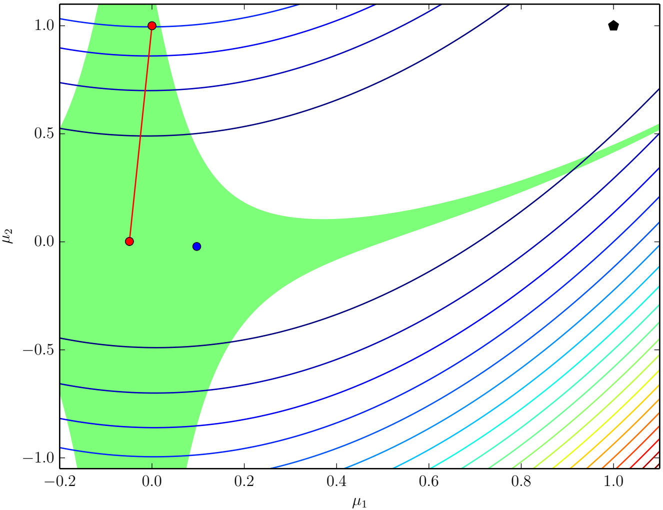

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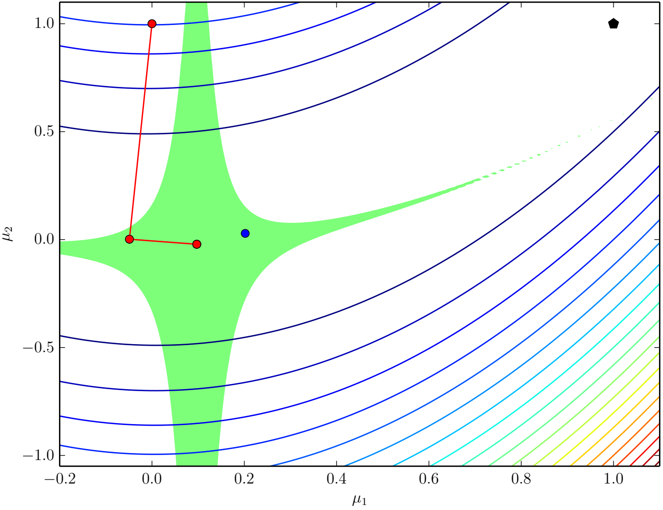

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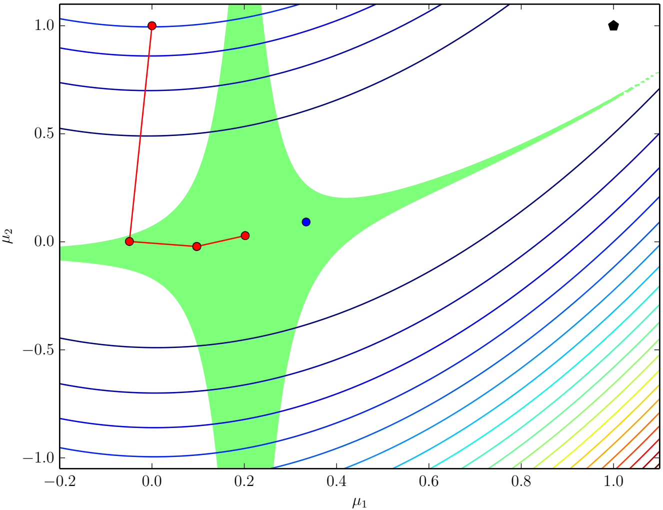

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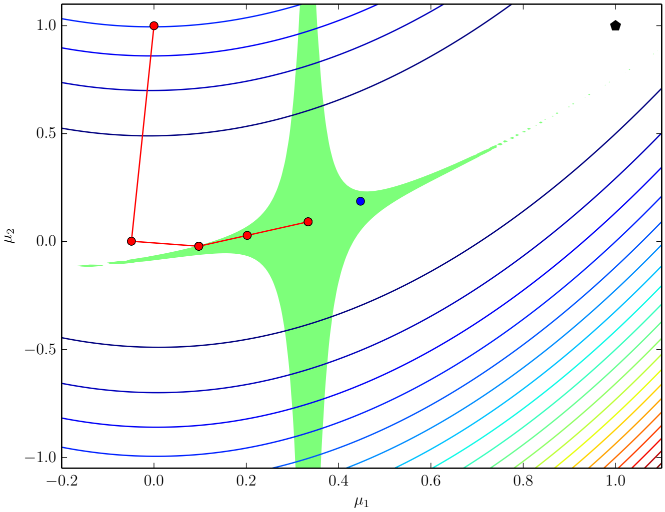

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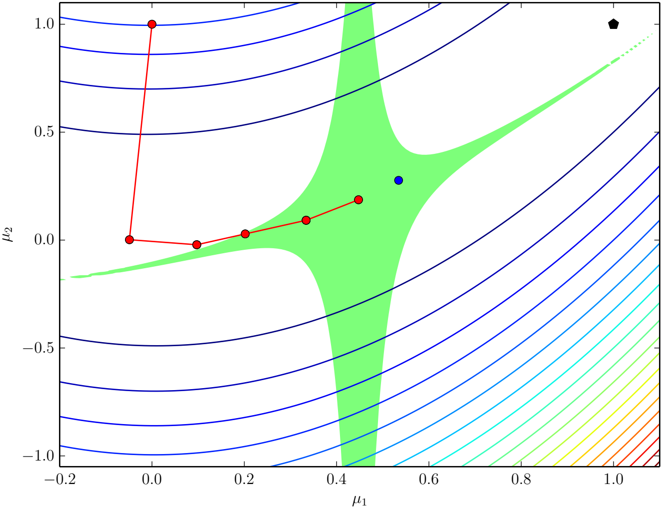

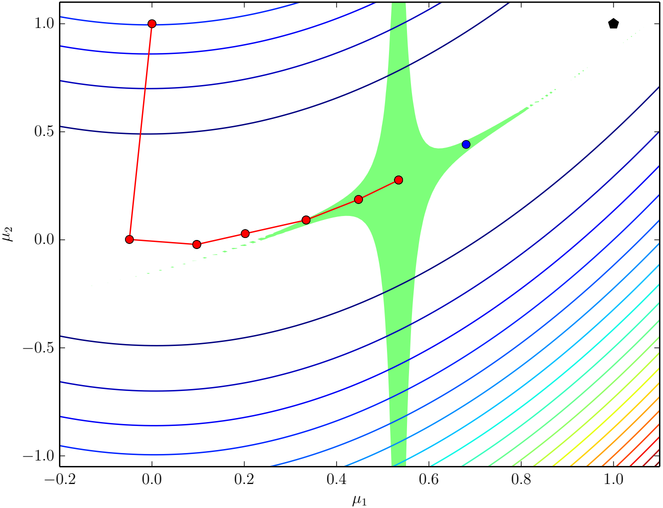
1.0
0.5
0.0
−0.5
−1.0
μ_2
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
μ_1

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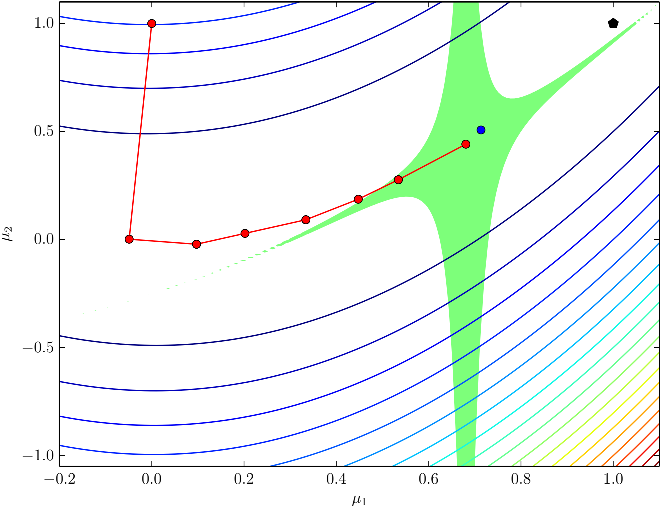

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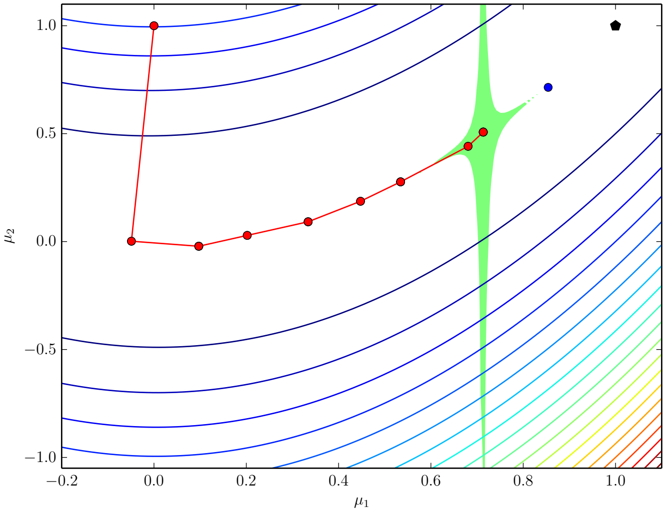

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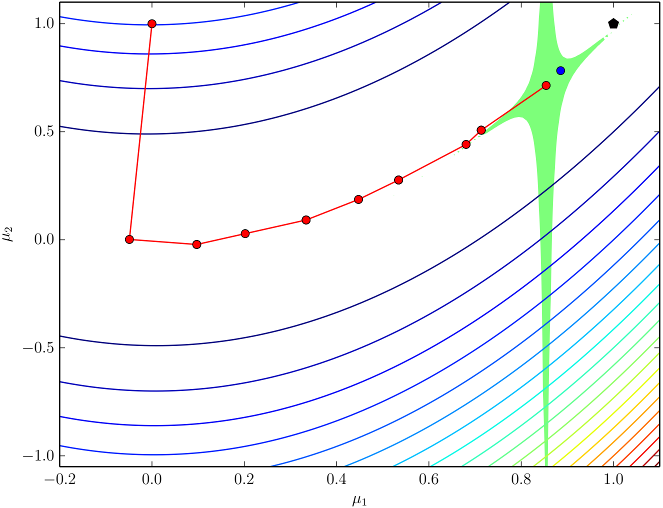

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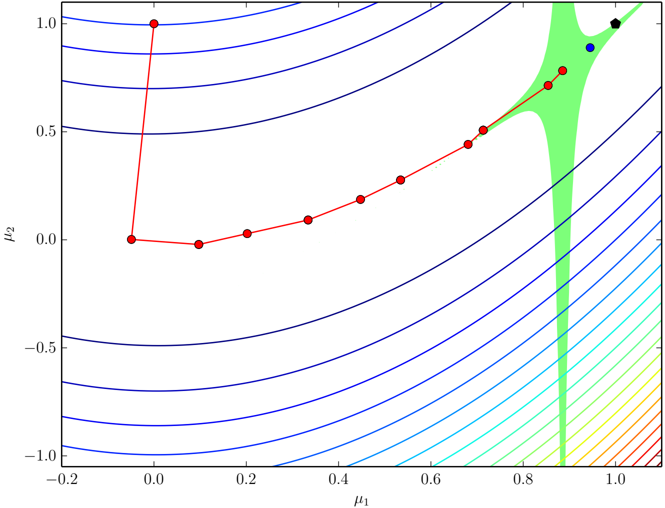

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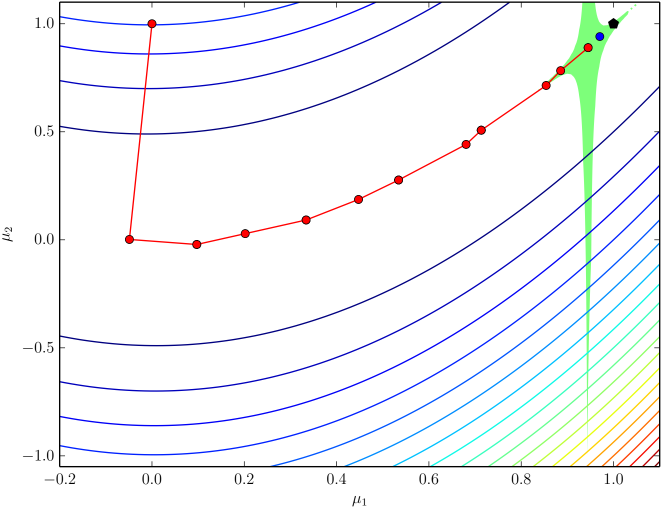

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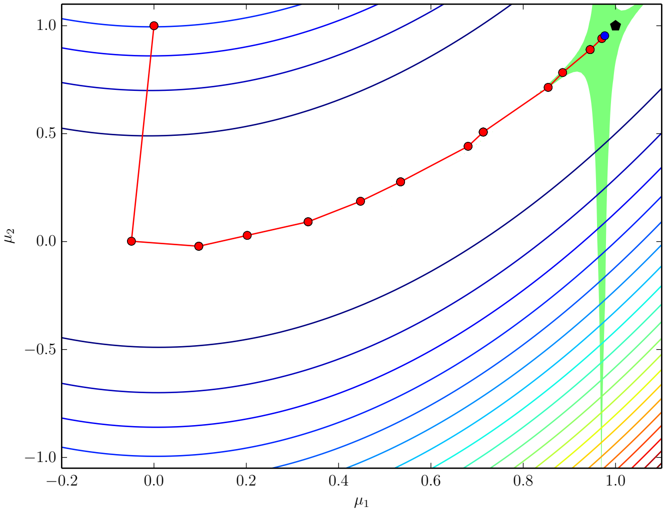

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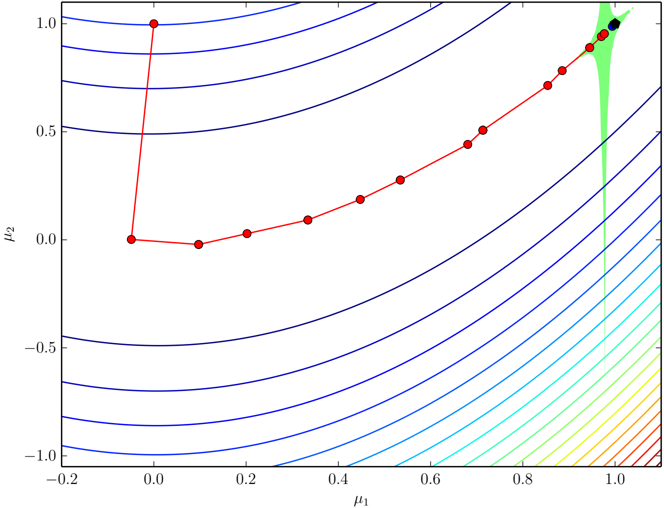
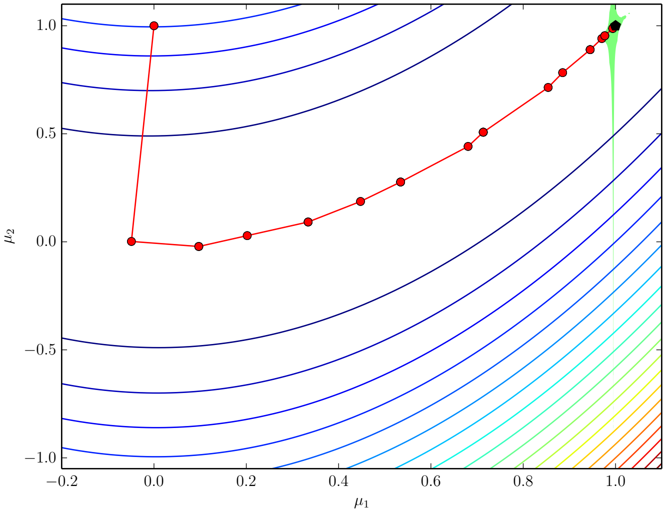


A look at error-aware trust regions



Trust region ingredients for global convergence

Approximation models

$$m_k(\mu),\ \psi_k(\mu)$$

Error indicators

$$|F(\mu_k) - F(\mu) + m_k(\mu) - m_k(\mu_k)| \leq \zeta \vartheta_k(\mu) \qquad \zeta > 0$$

$$\|\nabla F(\mu) - \nabla m_k(\mu)\| \leq \xi \varphi_k(\mu) \qquad \xi > 0$$

$$|F(\mu_k) - F(\mu) + \psi_k(\mu) - \psi_k(\mu_k)| \leq \sigma \theta_k(\mu) \qquad \sigma > 0$$

Adaptivity

$$\vartheta_k(\mu_k) \leq \kappa_\vartheta \Delta_k$$

$$\varphi_k(\mu_k) \leq \kappa_\varphi \min\{\|\nabla m_k(\mu_k)\|,\ \Delta_k\}$$

$$\theta_k(\hat{\mu}_k)^\omega \leq \eta \min\{m_k(\mu_k) - m_k(\hat{\mu}_k),\ r_k\}$$

Global convergence

$$\liminf_{k \to \infty} \|\nabla F(\mu_k)\| = 0$$

Proposed approach: managed inexactness

Replace expensive PDE with inexpensive approximation model

- **Reduced-order models** used for *inexact PDE evaluations*
- **Partially converged solutions** used for *inexact PDE evaluations*
- **Anisotropic sparse grids** used for *inexact integration* of risk measures

$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad F(\mu) \qquad \longrightarrow \qquad \underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad m_k(\mu)$$

Manage inexactness with trust region method

- Embedded in globally convergent **trust region** method
- **Error indicators** to account for *all* sources of inexactness
- **Refinement** of approximation model using *greedy algorithms*

$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad F(\mu) \qquad \longrightarrow \qquad \begin{array}{ll} \underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} & m_k(\mu) \\ \text{subject to} & \|\mu - \mu_k\| \leq \Delta_k \end{array}$$

- Model reduction ansatz: *state vector lies in low-dimensional subspace*

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

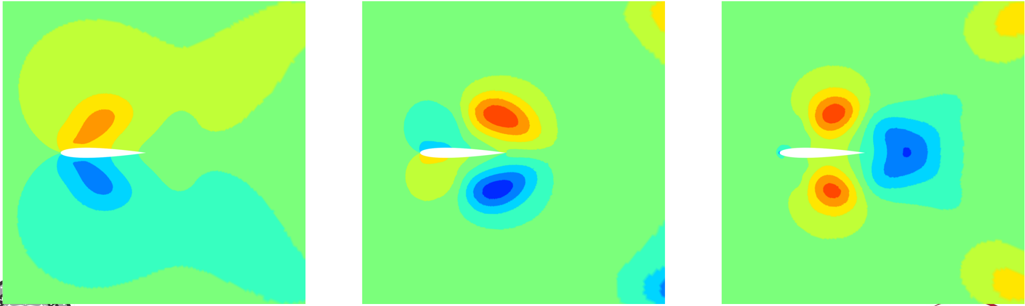
  - $\boldsymbol{\Phi} = \begin{bmatrix}\boldsymbol{\phi}^1 & \cdots & \boldsymbol{\phi}^{k_u}\end{bmatrix} \in \mathbb{R}^{n_u \times k_u}$ is the reduced (trial) basis ($n_u \gg k_u$)
  - $\mathbf{u}_r \in \mathbb{R}^{k_u}$ are the reduced coordinates of $\mathbf{u}$

- Substitute into $\mathbf{r}(\mathbf{u}, \boldsymbol{\mu}) = 0$ and project onto columnspace of a test basis $\boldsymbol{\Psi} \in \mathbb{R}^{n_u \times k_u}$ to obtain a square system

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

Few global, data-driven basis functions v. many local ones

- Instead of using traditional *local* shape functions, use **global shape functions**
- Instead of a-priori, analytical shape functions, leverage data-rich computing environment by using **data-driven modes**



Definition of $\boldsymbol{\Psi}$: minimum-residual reduced-order models

A ROM possesses the **minimum-residual property** if $\boldsymbol{\Psi}^T \mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r, \ \boldsymbol{\mu}) = 0$ is equivalent to the optimality condition of

$$\underset{\mathbf{u}_r \in \mathbb{R}^{k_\mathbf{u}}}{\text{minimize}} \quad \|\mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r, \ \boldsymbol{\mu})\|_{\boldsymbol{\Theta}} \qquad \boldsymbol{\Theta} \succ 0$$

which requires

$$\boldsymbol{\Psi}(\mathbf{u}, \ \boldsymbol{\mu}) = \boldsymbol{\Theta} \frac{\partial \mathbf{r}}{\partial \mathbf{u}}(\mathbf{u}, \ \boldsymbol{\mu}) \boldsymbol{\Phi}$$

Definition of Ψ: minimum-residual reduced-order models

A ROM possesses the **minimum-residual property** if $\boldsymbol{\Psi}^T \mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r,\ \boldsymbol{\mu}) = 0$ is equivalent to the optimality condition of

$$\underset{\mathbf{u}_r \in \mathbb{R}^{k_\mathbf{u}}}{\text{minimize}} \quad \|\mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r,\ \boldsymbol{\mu})\|_{\boldsymbol{\Theta}} \qquad \boldsymbol{\Theta} \succ 0$$

which requires

$$\boxed{\boldsymbol{\Psi}(\mathbf{u},\ \boldsymbol{\mu}) = \boldsymbol{\Theta} \frac{\partial \mathbf{r}}{\partial \mathbf{u}}(\mathbf{u},\ \boldsymbol{\mu}) \boldsymbol{\Phi}}$$

Implications of the minimum-residual property

- ("Optimality") For any $\mathbf{u} \in \text{col}(\boldsymbol{\Phi})$,

$$\|\mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r,\ \boldsymbol{\mu})\|_{\boldsymbol{\Theta}} \leq \|\mathbf{r}(\mathbf{u},\ \boldsymbol{\mu})\|_{\boldsymbol{\Theta}}$$

- (Monotonicity) For any $\text{col}(\boldsymbol{\Phi}') \subseteq \text{col}(\boldsymbol{\Phi})$,

$$\|\mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r,\ \boldsymbol{\mu})\|_{\boldsymbol{\Theta}} \leq \left\|\mathbf{r}(\boldsymbol{\Phi}'\mathbf{u}_r',\ \boldsymbol{\mu})\right\|_{\boldsymbol{\Theta}}$$

- (Interpolation) If $\mathbf{u}(\boldsymbol{\mu}) \in \text{col}(\boldsymbol{\Phi})$, then

$$\mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r,\ \boldsymbol{\mu}) = 0 \qquad \text{and} \qquad \mathbf{u}(\boldsymbol{\mu}) = \boldsymbol{\Phi}\mathbf{u}_r$$

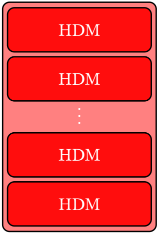
Offline-online approach to optimization with ROMs

Schematic

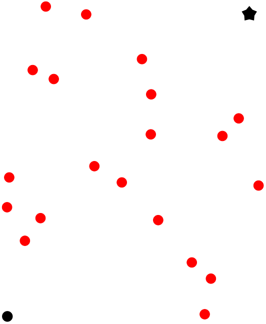
μ-space

Breakdown of Computational Effort

Offline-online approach to optimization with ROMs



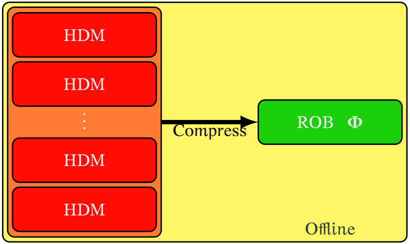
Schematic



μ-space

Breakdown of Computational Effort

Offline-online approach to optimization with ROMs



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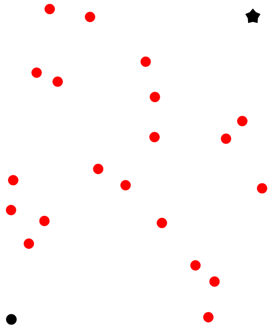

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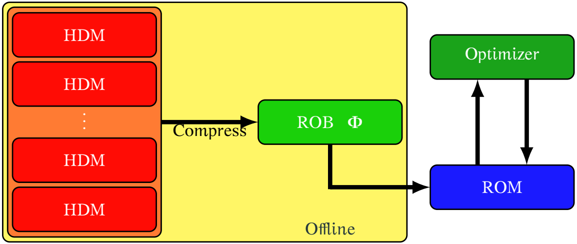

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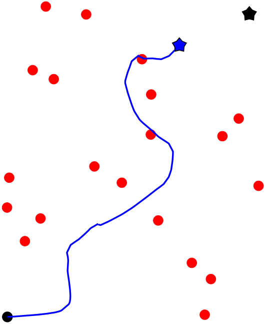

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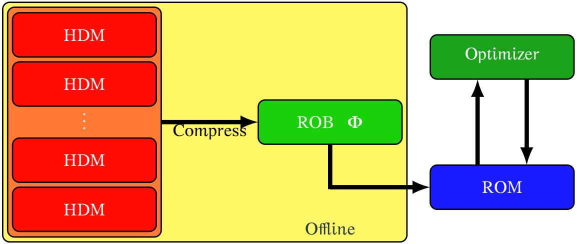
Offline-online approach to optimization with ROMs



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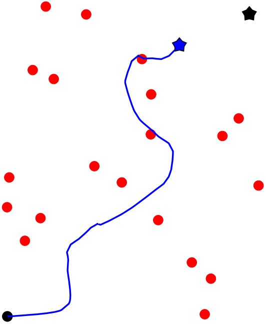


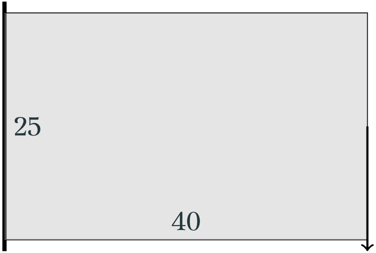
μ-space

Breakdown of Computational Effort

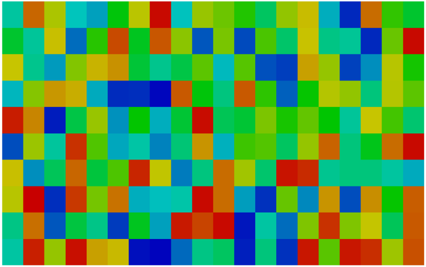
No convergence **Scales exponentially with N_μ**

Numerical demonstration: offline-online breakdown

- *Greedy* Training
  - 5000 candidate points (LHS)
  - 50 snapshots
  - Error indicator: $\|\mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r, \boldsymbol{\mu})\|$
- State reduction ($\boldsymbol{\Phi}$)
  - POD
  - $k_u = 25$
  - Polynomialization acceleration

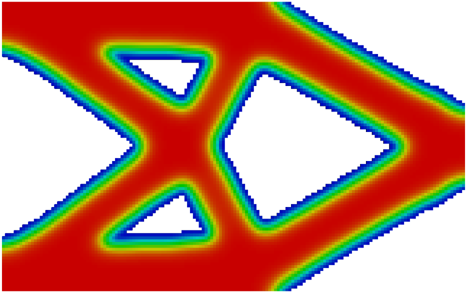


Stiffness maximization, volume constraint

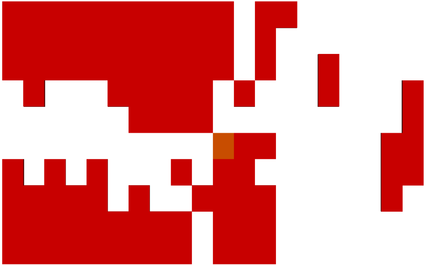


Parametrization with $n_\mu = 200$

Numerical demonstration: offline-online breakdown



Optimal Solution
(1.97×10^4 s)



ROM Solution

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

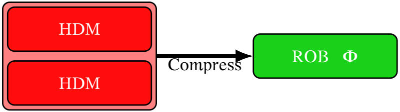
Trust region framework for optimization with ROMs

Schematic

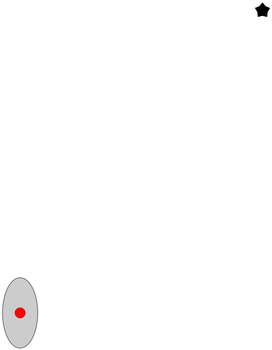
μ-space

Breakdown of Computational Effort

Trust region framework for optimization with ROMs



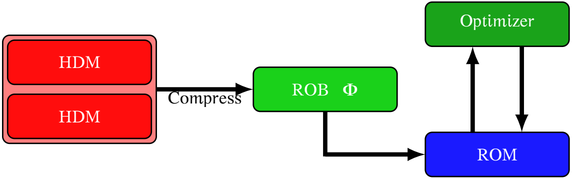
Schematic



μ-space

Breakdown of Computational Effort

Trust region framework for optimization with ROMs



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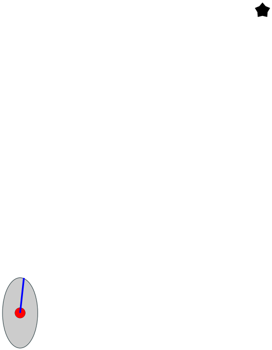

μ-space

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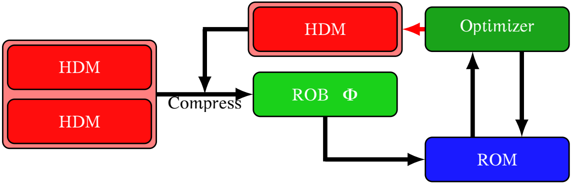

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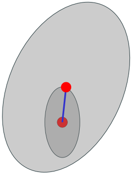

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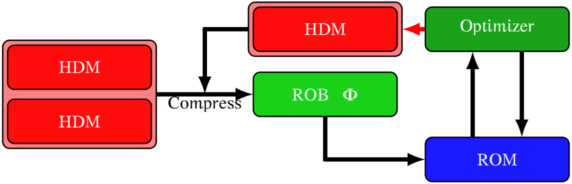

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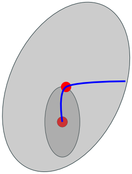

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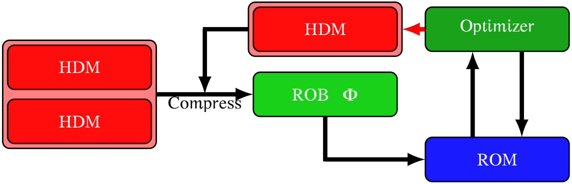

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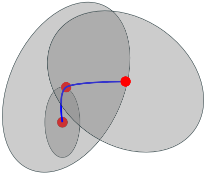

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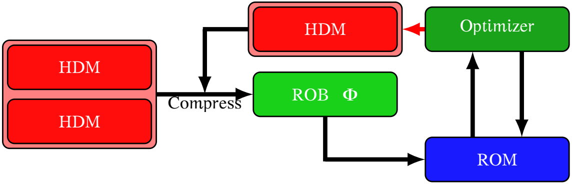

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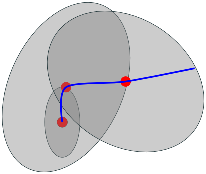

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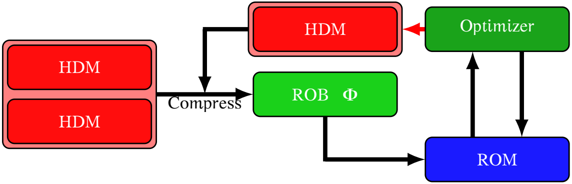

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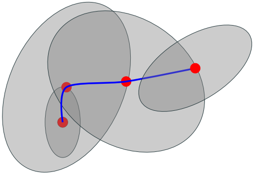

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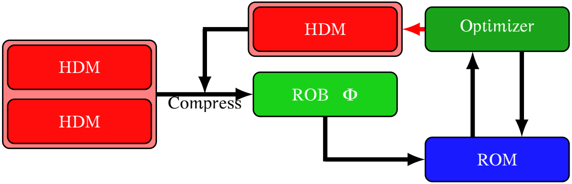

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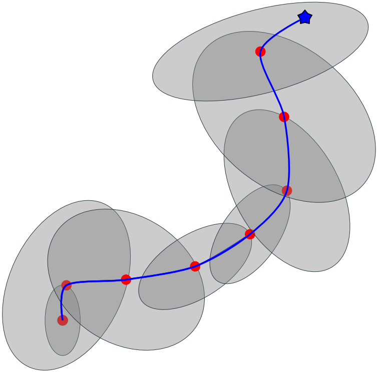

μ-space

Breakdown of Computational Effort

Trust region ingredients for global convergence

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Adaptivity

$$\vartheta_k(\mu_k) \le \kappa_\vartheta \Delta_k$$
$$\varphi_k(\mu_k) \le \kappa_\varphi \min\{\|\nabla m_k(\mu_k)\|,\ \Delta_k\}$$
$$\theta_k(\hat{\mu}_k)^\omega \le \eta \min\{m_k(\mu_k) - m_k(\hat{\mu}_k),\ r_k\}$$

Global convergence

$$\liminf_{k\to\infty} \|\nabla F(\mu_k)\| = 0$$

Trust region method: ROM approximation model

Approximation models based on reduced-order models

$$m_k(\mu) = \mathcal{J}(\Phi_k u_r(\mu), \mu) \qquad \psi_k(\mu) = \mathcal{J}(u(\mu), \mu)$$

Error indicators from residual-based error bounds

$$\vartheta_k(\mu) = \|r(\Phi_k u_r(\mu_k), \mu_k)\|_\Theta + \|r(\Phi_k u_r(\mu), \mu)\|_\Theta$$

$$\varphi_k(\mu) = \|r(\Phi_k u_r(\mu), \mu)\|_\Theta + \left\|r^\lambda(\Phi_k u_r(\mu), \Psi_k \lambda_r(\mu), \mu)\right\|_{\Theta^\lambda}$$

$$\theta_k(\mu) = 0$$

Adaptivity to refine basis at trust region center

$$\Phi_k = \begin{bmatrix} u(\mu_k) & \lambda(\mu_k) & \mathtt{POD}(U_k) & \mathtt{POD}(V_k) \end{bmatrix}$$

$$U_k = \begin{bmatrix} u(\mu_0) & \cdots & u(\mu_{k-1}) \end{bmatrix} \qquad V_k = \begin{bmatrix} \lambda(\mu_0) & \cdots & \lambda(\mu_{k-1}) \end{bmatrix}$$

$$\text{Interpolation property} \implies \vartheta_k(\mu_k) = \varphi_k(\mu_k) = 0$$

Trust region method: ROM approximation model

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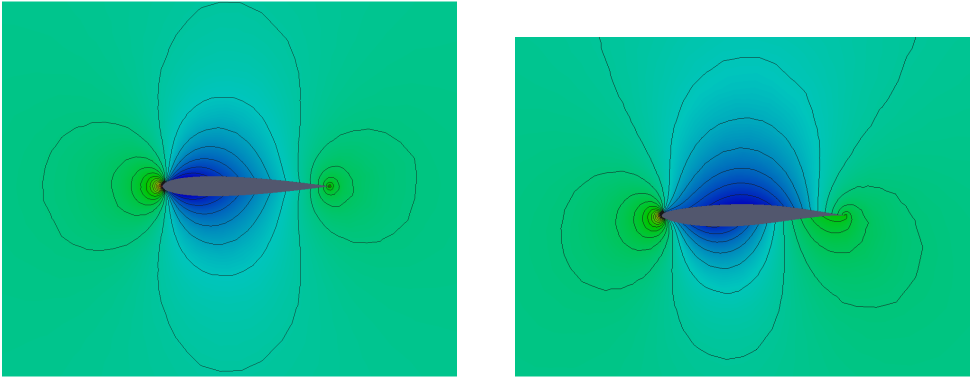
$$\liminf_{k\to\infty} \|\nabla \mathcal{J}(u(\mu_k), \mu_k)\| = 0$$

Compressible, inviscid airfoil design

Pressure discrepancy minimization (Euler equations)

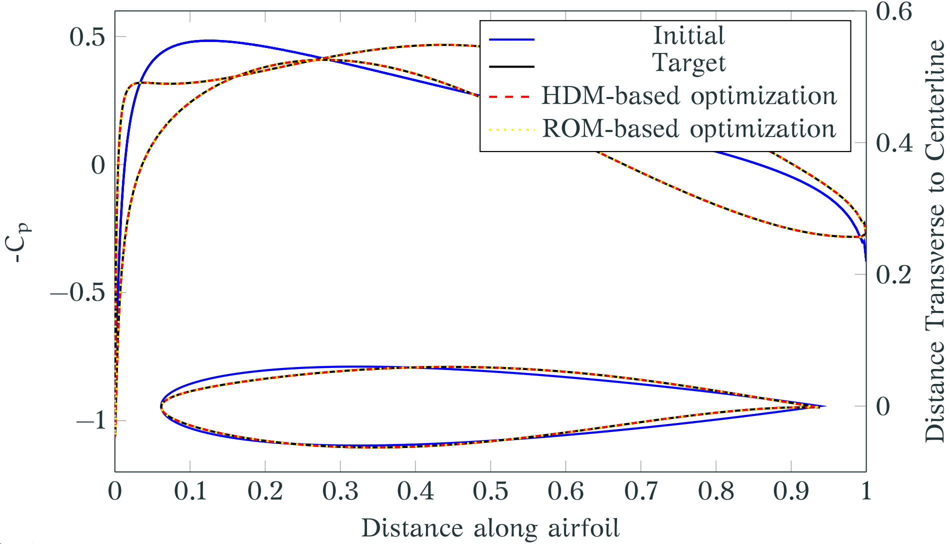


NACA0012: Initial

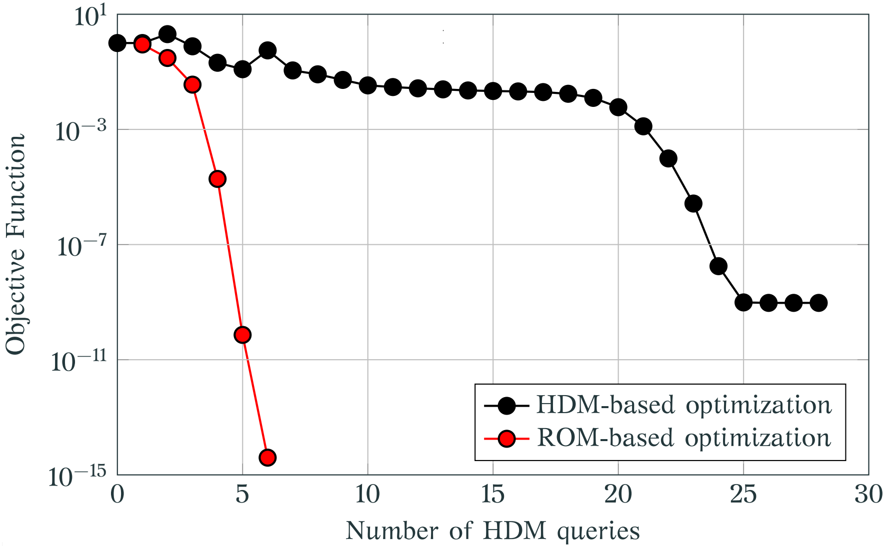
RAE2822: Target

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

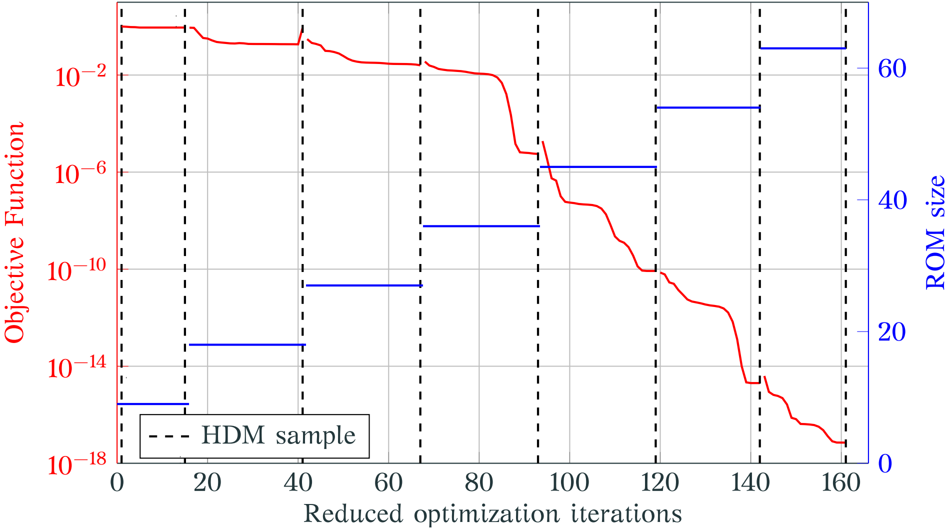
Proposed method: recovers target airfoil



Proposed method: 4× fewer HDM queries



At the cost of ROM queries

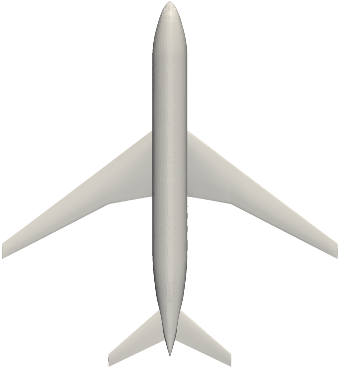


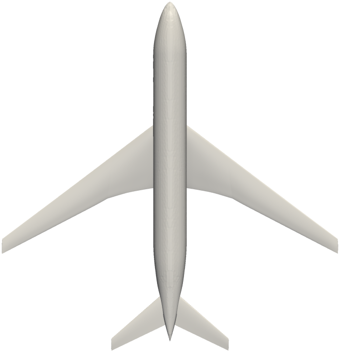
Shape optimization of aircraft in turbulent flow

$$\underset{\mu \in \mathbb{R}^4}{\text{minimize}} \quad -L_z(\mu)/L_x(\mu)$$
$$\text{subject to} \quad L_z(\mu) = \bar{L}_z$$

- **Flow**: $M = 0.85 \quad \alpha = 2.32^\circ \quad Re = 5 \times 10^6$
- **Equations**: RANS with Spalart-Allmaras
- **Solver**: Vertex-centered finite volume method
- **Mesh**: **11.5M** nodes, **68M** tetra, **69M** DOF

$$\mu = [\mathbf{L} \quad r_x \quad \phi \quad r_z]$$





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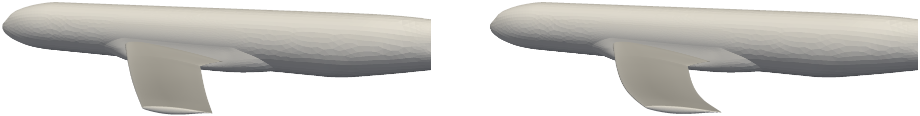
$$\mu = [L \quad \mathbf{r_x} \quad \phi \quad r_z]$$



Localized sweep

Shape optimization of aircraft in turbulent flow

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$$\text{subject to} \quad L_z(\mu) = \bar{L}_z$$

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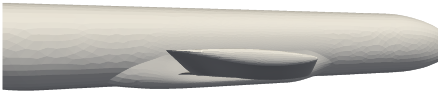
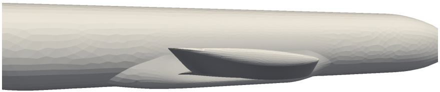
- **Mesh**: **11.5M** nodes, **68M** tetra, **69M** DOF

$$\mu = [L \quad r_x \quad \phi \quad r_z]$$





Twist

Shape optimization of aircraft in turbulent flow

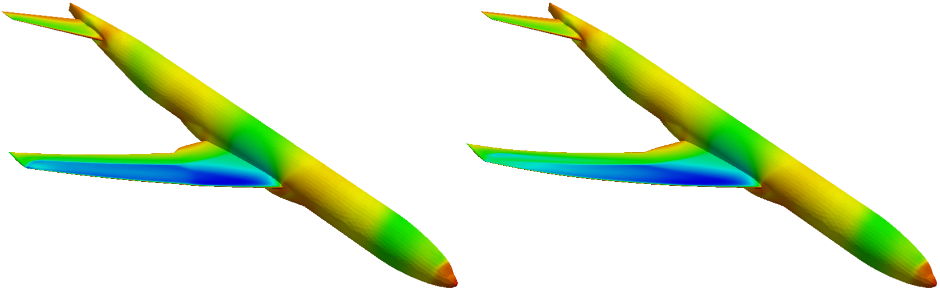
$$\underset{\mu \in \mathbb{R}^4}{\text{minimize}} \quad -L_z(\mu)/L_x(\mu)$$
$$\text{subject to} \quad L_z(\mu) = \bar{L}_z$$

- **Flow**: $M = 0.85 \quad \alpha = 2.32^\circ \quad Re = 5 \times 10^6$
- **Equations**: RANS with Spalart-Allmaras
- **Solver**: Vertex-centered finite volume method
- **Mesh**: **11.5M** nodes, **68M** tetra, **69M** DOF

$$\mu = [L \quad r_x \quad \phi \quad \mathbf{r_z}]$$

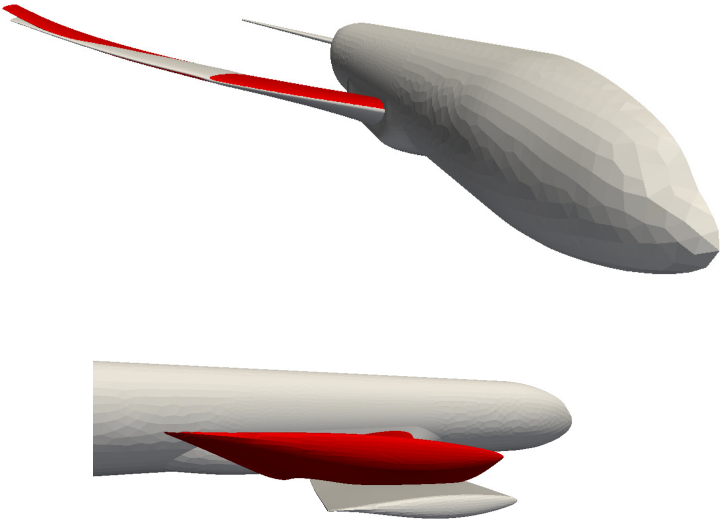
Localized dihedral

Optimized shape: reduction in 2.2 drag counts



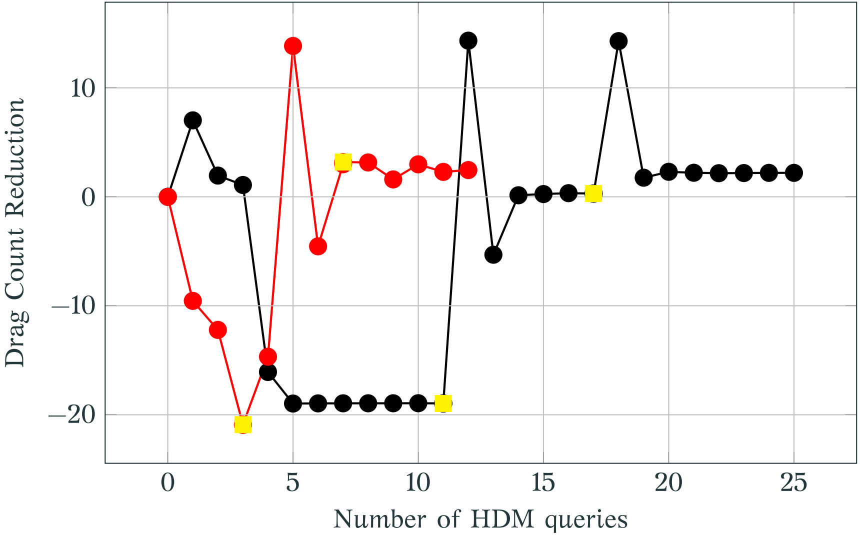
Baseline (left) and optimized (right) shape – colored by C_p

Optimized shape: reduction in 2.2 drag counts



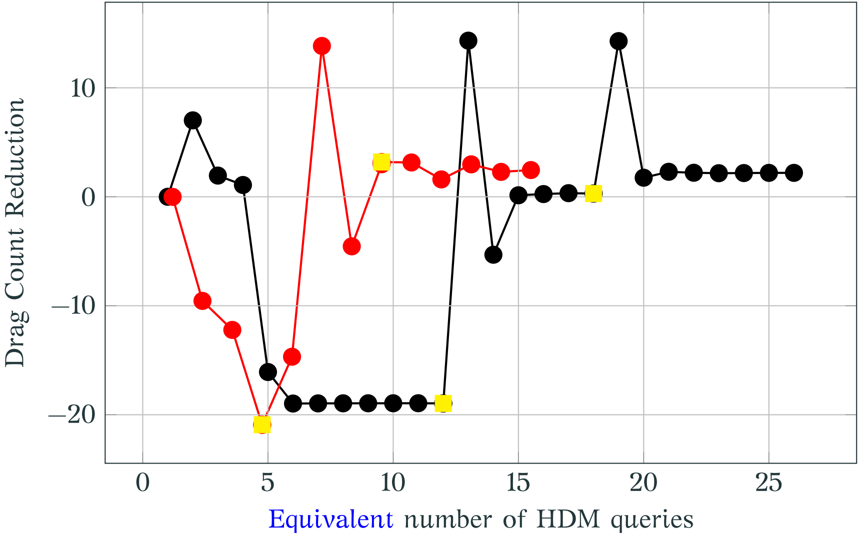
Baseline (gray) and optimized shape (red) – 2× magnification

Proposed method: 2x reduction in number of HDM queries



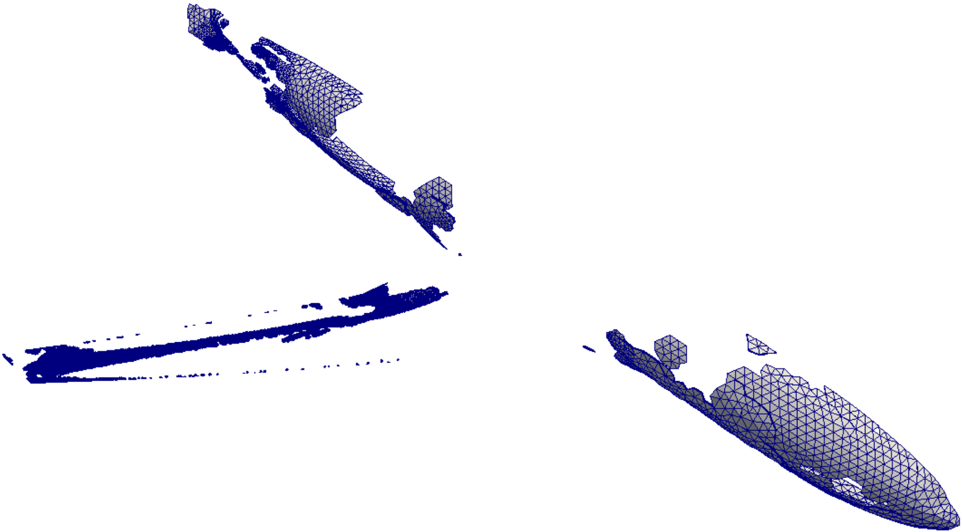
(—●—) HDM optimization, (—●—) ROM optimization,
(■) Augmented Lagrangian update

Proposed method: 1.6x reduction in overall cost



(—●—) HDM optimization, (—●—) ROM optimization,
(■) Augmented Lagrangian update

Sample mesh has 0.6% the nodes of the full mesh



The sample mesh at an intermediate iteration with **72k nodes**
(vs. the full mesh with **11.5M nodes**)

Stochastic PDE-constrained optimization formulation

$$\begin{aligned} \underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad & \mathbb{E}[\mathcal{J}(\mathbf{u}, \boldsymbol{\mu}, \cdot)] \\ \text{subject to} \quad & \mathbf{r}(\mathbf{u}; \boldsymbol{\mu}, \boldsymbol{\xi}) = 0 \quad \forall \boldsymbol{\xi} \in \boldsymbol{\Xi} \end{aligned}$$

- $\mathbf{r} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \times \mathbb{R}^{n_\xi} \to \mathbb{R}^{n_u}$ discretized stochastic PDE
- $\mathcal{J} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \times \mathbb{R}^{n_\xi} \to \mathbb{R}$ quantity of interest
- $\mathbf{u} \in \mathbb{R}^{n_u}$ PDE state vector
- $\boldsymbol{\mu} \in \mathbb{R}^{n_\mu}$ (deterministic) optimization parameters
- $\boldsymbol{\xi} \in \mathbb{R}^{n_\xi}$ stochastic parameters
- $\mathbb{E}[\mathcal{F}] \equiv \int_{\boldsymbol{\Xi}} \mathcal{F}(\boldsymbol{\xi})\rho(\boldsymbol{\xi})\, d\boldsymbol{\xi}$

First source of inexactness: anisotropic sparse grids

Stochastic collocation using anisotropic sparse grid nodes to approximate integral with summation

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

$$\Downarrow$$

$$\begin{aligned} \underset{\mathbf{u}\in\mathbb{R}^{n_\mathbf{u}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_\boldsymbol{\mu}}}{\text{minimize}} \quad & \mathbb{E}_\mathcal{I}[\mathcal{J}(\mathbf{u},\boldsymbol{\mu},\cdot)] \\ \text{subject to} \quad & \mathbf{r}(\mathbf{u},\boldsymbol{\mu},\boldsymbol{\xi}) = 0 \quad \forall \boldsymbol{\xi} \in \boldsymbol{\Xi}_\mathcal{I} \end{aligned}$$

[Kouri et al., 2013, Kouri et al., 2014]

Second source of inexactness: reduced-order models

Stochastic collocation of the reduced-order model over anisotropic sparse grid nodes used to approximate integral with cheap summation

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

$$\Downarrow$$

$$\begin{aligned} \underset{\mathbf{u}\in\mathbb{R}^{n_\mathbf{u}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_\boldsymbol{\mu}}}{\text{minimize}} \quad & \mathbb{E}_\mathcal{I}[\mathcal{J}(\mathbf{u},\ \boldsymbol{\mu},\ \cdot\ )] \\ \text{subject to} \quad & \mathbf{r}(\mathbf{u},\ \boldsymbol{\mu},\ \boldsymbol{\xi}) = 0 \quad \forall \boldsymbol{\xi} \in \boldsymbol{\Xi}_\mathcal{I} \end{aligned}$$

$$\Downarrow$$

$$\begin{aligned} \underset{\mathbf{u}_r\in\mathbb{R}^{k_\mathbf{u}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_\boldsymbol{\mu}}}{\text{minimize}} \quad & \mathbb{E}_\mathcal{I}[\mathcal{J}(\boldsymbol{\Phi}\mathbf{u}_r,\ \boldsymbol{\mu},\ \cdot\ )] \\ \text{subject to} \quad & \boldsymbol{\Psi}^T\mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r,\ \boldsymbol{\mu},\ \boldsymbol{\xi}) = 0 \quad \forall \boldsymbol{\xi} \in \boldsymbol{\Xi}_\mathcal{I} \end{aligned}$$

Proposed approach: managed inexactness

Replace expensive PDE with inexpensive approximation model

- **Reduced-order models** used for *inexact PDE evaluations*
- **Partially converged solutions** used for *inexact PDE evaluations*
- **Anisotropic sparse grids** used for *inexact integration* of risk measures

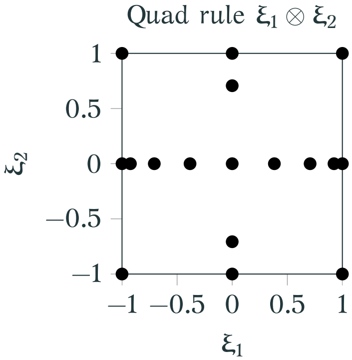
$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad F(\mu) \qquad \longrightarrow \qquad \underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad m_k(\mu)$$

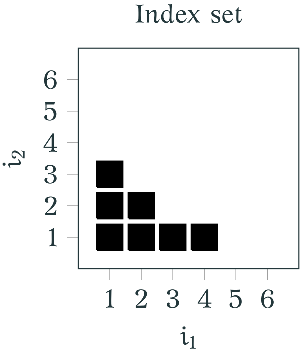
Manage inexactness with trust region method

- Embedded in globally convergent **trust region** method
- **Error indicators** to account for *all* sources of inexactness
- **Refinement** of approximation model using *greedy algorithms*

$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad F(\mu) \qquad \longrightarrow \qquad \begin{aligned} &\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} && m_k(\mu) \\ &\text{subject to} && \|\mu - \mu_k\| \leq \Delta_k \end{aligned}$$

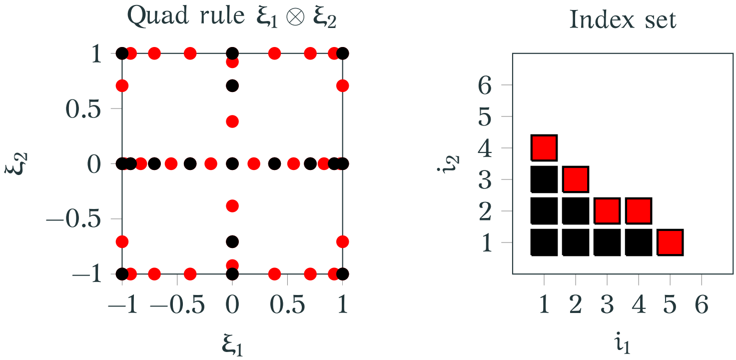
Source of inexactness: anisotropic sparse grids





Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

Source of inexactness: anisotropic sparse grids



Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

Trust region method: ROM/SG approximation model

Approximation models built on two sources of inexactness

$$m_k(\mu) = \mathbb{E}_{\mathcal{I}_k}\left[\mathcal{J}(\Phi_k u_r(\mu,\cdot),\mu,\cdot)\right]$$
$$\psi_k(\mu) = \mathbb{E}_{\mathcal{I}_k'}\left[\mathcal{J}(\Phi_k' u_r(\mu,\cdot),\mu,\cdot)\right]$$

Error indicators that account for both sources of error

$$\vartheta_k(\mu) = ||\mu - \mu_k||$$
$$\varphi_k(\mu) = \alpha_1 \mathcal{E}_1(\mu;\mathcal{I}_k,\Phi_k) + \alpha_2 \mathcal{E}_2(\mu;\mathcal{I}_k,\Phi_k) + \alpha_3 \mathcal{E}_4(\mu;\mathcal{I}_k,\Phi_k)$$
$$\theta_k(\mu) = \beta_1(\mathcal{E}_1(\mu;\mathcal{I}_k',\Phi_k') + \mathcal{E}_1(\mu_k;\mathcal{I}_k',\Phi_k')) + \beta_2(\mathcal{E}_3(\mu;\mathcal{I}_k',\Phi_k') + \mathcal{E}_3(\mu_k;\mathcal{I}_k',\Phi_k'))$$

Reduced-order model errors

$$\mathcal{E}_1(\mu;\mathcal{I},\Phi) = \mathbb{E}_{\mathcal{I}\cup\mathcal{N}(\mathcal{I})}\left[||\mathbf{r}(\Phi u_r(\mu,\cdot),\mu,\cdot)||\right]$$
$$\mathcal{E}_2(\mu;\mathcal{I},\Phi) = \mathbb{E}_{\mathcal{I}\cup\mathcal{N}(\mathcal{I})}\left[\left|\left|\mathbf{r}^{\lambda}(\Phi u_r(\mu,\cdot),\Psi\lambda_r(\mu,\cdot),\mu,\cdot)\right|\right|\right]$$

Sparse grid truncation errors

$$\mathcal{E}_3(\mu;\mathcal{I},\Phi) = \mathbb{E}_{\mathcal{N}(\mathcal{I})}\left[|\mathcal{J}(\Phi u_r(\mu,\cdot),\mu,\cdot)|\right]$$
$$\mathcal{E}_4(\mu;\mathcal{I},\Phi) = \mathbb{E}_{\mathcal{N}(\mathcal{I})}\left[||\nabla\mathcal{J}(\Phi u_r(\mu,\cdot),\mu,\cdot)||\right]$$

Final requirement for convergence: Adaptivity

With the approximation model, $m_k(\mu)$, and gradient error indicator, $\varphi_k(\mu)$

$$\begin{aligned} m_k(\mu) &= \mathbb{E}_{\mathcal{I}_k}\left[\mathcal{J}(\Phi_k u_r(\mu, \cdot), \mu, \cdot)\right] \\ \varphi_k(\mu) &= \alpha_1 \mathcal{E}_1(\mu; \mathcal{I}_k, \Phi_k) + \alpha_2 \mathcal{E}_2(\mu; \mathcal{I}_k, \Phi_k) + \alpha_3 \mathcal{E}_4(\mu; \mathcal{I}_k, \Phi_k) \end{aligned}$$

the sparse grid $\mathcal{I}_k$ and reduced-order basis Φ_k must be constructed such that the gradient condition holds

$$\varphi_k(\mu_k) \leq \kappa_\varphi \min\{||\nabla m_k(\mu_k)||, \Delta_k\}$$

Define dimension-adaptive greedy method to target each source of error such that the stronger conditions hold

$$\begin{aligned} \mathcal{E}_1(\mu_k; \mathcal{I}, \Phi) &\leq \frac{\kappa_\varphi}{3\alpha_1} \min\{||\nabla m_k(\mu_k)||, \Delta_k\} \\ \mathcal{E}_2(\mu_k; \mathcal{I}, \Phi) &\leq \frac{\kappa_\varphi}{3\alpha_2} \min\{||\nabla m_k(\mu_k)||, \Delta_k\} \\ \mathcal{E}_4(\mu_k; \mathcal{I}, \Phi) &\leq \frac{\kappa_\varphi}{3\alpha_3} \min\{||\nabla m_k(\mu_k)||, \Delta_k\} \end{aligned}$$

Adaptivity: Dimension-adaptive greedy method

while $\mathcal{E}_4(\boldsymbol{\Phi}, \mathcal{I}, \boldsymbol{\mu}_k) > \frac{\kappa_\varphi}{3\alpha_3} \min\{||\nabla m_k(\boldsymbol{\mu}_k)||, \Delta_k\}$ **do**

Refine index set: Dimension-adaptive sparse grids

$$\mathcal{I}_k \leftarrow \mathcal{I}_k \cup \{\mathbf{j}^*\} \qquad \text{where} \qquad \mathbf{j}^* = \underset{\mathbf{j} \in \mathcal{N}(\mathcal{I}_k)}{\arg\max}\ \mathbb{E}_{\mathbf{j}}\left[||\nabla \mathcal{J}(\boldsymbol{\Phi}\mathbf{u}_r(\boldsymbol{\mu}, \cdot), \boldsymbol{\mu}, \cdot)||\right]$$

Adaptivity: Dimension-adaptive greedy method

while $\mathcal{E}_4(\boldsymbol{\Phi}, \mathcal{I}, \boldsymbol{\mu}_k) > \frac{\kappa_\varphi}{3\alpha_3} \min\{\|\nabla m_k(\boldsymbol{\mu}_k)\|, \Delta_k\}$ **do**

Refine index set: Dimension-adaptive sparse grids

$$\mathcal{I}_k \leftarrow \mathcal{I}_k \cup \{\mathbf{j}^*\} \qquad \text{where} \qquad \mathbf{j}^* = \arg\max_{\mathbf{j}\in\mathcal{N}(\mathcal{I}_k)} \mathbb{E}_{\mathbf{j}}\left[\|\nabla\mathcal{J}(\boldsymbol{\Phi}\mathbf{u}_r(\boldsymbol{\mu}, \cdot), \boldsymbol{\mu}, \cdot)\|\right]$$

Refine reduced-order basis: Greedy sampling

while $\mathcal{E}_1(\boldsymbol{\Phi}, \mathcal{I}, \boldsymbol{\mu}_k) > \frac{\kappa_\varphi}{3\alpha_1} \min\{\|\nabla m_k(\boldsymbol{\mu}_k)\|, \Delta_k\}$ **do**

$$\boldsymbol{\Phi}_k \leftarrow \begin{bmatrix} \boldsymbol{\Phi}_k & \mathbf{u}(\boldsymbol{\mu}_k, \boldsymbol{\xi}^*) & \boldsymbol{\lambda}(\boldsymbol{\mu}_k, \boldsymbol{\xi}^*) \end{bmatrix}$$

$$\boldsymbol{\xi}^* = \arg\max_{\boldsymbol{\xi}\in\Xi_{\mathbf{j}^*}} \rho(\boldsymbol{\xi}) \|\mathbf{r}(\boldsymbol{\Phi}_k\mathbf{u}_r(\boldsymbol{\mu}_k, \boldsymbol{\xi}), \boldsymbol{\mu}_k, \boldsymbol{\xi})\|$$

end while

Adaptivity: Dimension-adaptive greedy method

while $\mathcal{E}_4(\boldsymbol{\Phi}, \mathcal{I}, \mu_k) > \frac{\kappa_\varphi}{3\alpha_3} \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$ **do**

Refine index set: Dimension-adaptive sparse grids

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Refine reduced-order basis: Greedy sampling

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$$\boldsymbol{\Phi}_k \leftarrow \begin{bmatrix} \boldsymbol{\Phi}_k & \mathbf{u}(\mu_k, \xi^*) & \boldsymbol{\lambda}(\mu_k, \xi^*) \end{bmatrix}$$

$$\xi^* = \underset{\xi \in \Xi_{\mathbf{j}^*}}{\arg\max}\ \rho(\xi)\, \|\mathbf{r}(\boldsymbol{\Phi}_k \mathbf{u}_r(\mu_k, \xi), \mu_k, \xi)\|$$

end while

while $\mathcal{E}_2(\boldsymbol{\Phi}, \mathcal{I}, \mu_k) > \frac{\kappa_\varphi}{3\alpha_2} \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$ **do**

$$\boldsymbol{\Phi}_k \leftarrow \begin{bmatrix} \boldsymbol{\Phi}_k & \mathbf{u}(\mu_k, \xi^*) & \boldsymbol{\lambda}(\mu_k, \xi^*) \end{bmatrix}$$

$$\xi^* = \underset{\xi \in \Xi_{\mathbf{j}^*}}{\arg\max}\ \rho(\xi)\, \left\|\mathbf{r}^{\boldsymbol{\lambda}}(\boldsymbol{\Phi}_k \mathbf{u}_r(\mu_k, \xi), \boldsymbol{\Psi}_k \boldsymbol{\lambda}_r(\mu_k, \xi), \mu_k, \xi)\right\|$$

end while

Optimal control of steady Burgers' equation

- **Optimization problem:**

$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad \int_\Xi \rho(\xi) \left[\int_0^1 \frac{1}{2} (u(\mu, \xi, x) - \bar{u}(x))^2 \, dx + \frac{\alpha}{2} \int_0^1 z(\mu, x)^2 \, dx \right] d\xi$$

where $u(\mu, \xi, x)$ solves

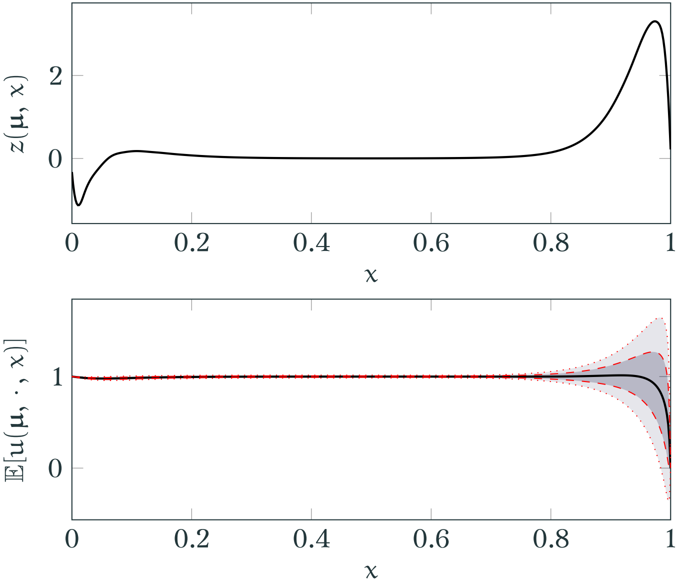
$$-\nu(\xi) \partial_{xx} u(\mu, \xi, x) + u(\mu, \xi, x) \partial_x u(\mu, \xi, x) = z(\mu, x) \quad x \in (0, 1), \quad \xi \in \Xi$$
$$u(\mu, \xi, 0) = d_0(\xi) \qquad u(\mu, \xi, 1) = d_1(\xi)$$

- **Target state:** $\bar{u}(x) \equiv 1$
- **Stochastic Space:** $\Xi = [-1, 1]^3$, $\rho(\xi) d\xi = 2^{-3} d\xi$

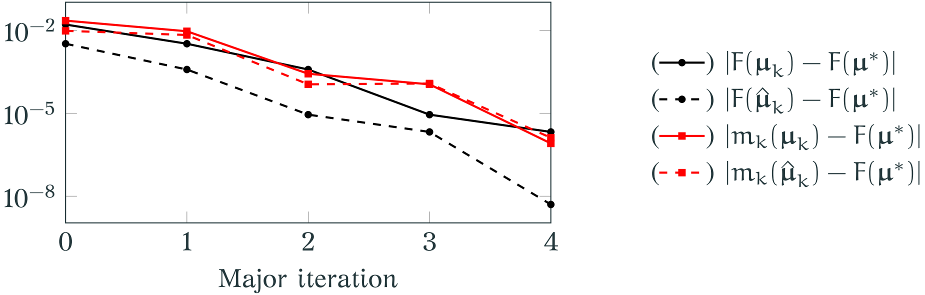
$$\nu(\xi) = 10^{\xi_1 - 2} \qquad d_0(\xi) = 1 + \frac{\xi_2}{1000} \qquad d_1(\xi) = \frac{\xi_3}{1000}$$

- **Parametrization:** $z(\mu, x)$ – cubic splines with 51 knots, $n_\mu = 53$

Optimal control and statistics



Optimal control and corresponding mean state (——) ± one (- - -) and two (·····) standard deviations

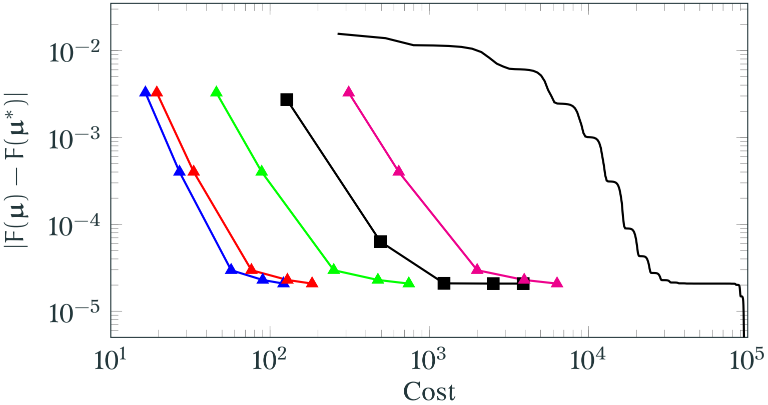


$F(\mu_k)$	$m_k(\mu_k)$	$F(\hat{\mu}_k)$	$m_k(\hat{\mu}_k)$	$\|\nabla F(\mu_k)\|$	ρ_k	Success?
6.6506e-02	7.2694e-02	5.3655e-02	5.9922e-02	2.2959e-02	1.0257e+00	1.0000e+00
5.3655e-02	5.9593e-02	5.0783e-02	5.7152e-02	2.3424e-03	9.7512e-01	1.0000e+00
5.0783e-02	5.0670e-02	5.0412e-02	5.0292e-02	1.9724e-03	9.8351e-01	1.0000e+00
5.0412e-02	5.0292e-02	5.0405e-02	5.0284e-02	9.2654e-05	8.7479e-01	1.0000e+00
5.0405e-02	5.0404e-02	5.0403e-02	5.0401e-02	8.3139e-05	9.9946e-01	1.0000e+00
5.0403e-02	5.0401e-02	-	-	2.2846e-06	-	-

Convergence history of trust region method built on two-level approximation

Significant reduction in cost, even if (largest) ROM only 10× faster than HDM

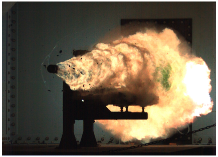
$$\text{Cost} = \text{nHdmPrim} + 0.5 \times \text{nHdmAdj} + \tau^{-1} \times (\text{nRomPrim} + 0.5 \times \text{nRomAdj})$$

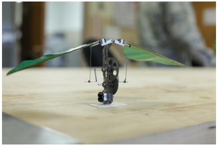


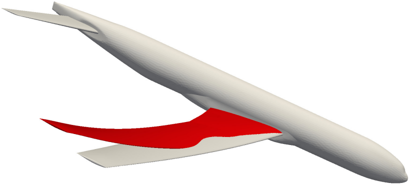
5-level isotropic SG (——), dimension-adaptive SG [Kouri et al., 2014] (—■—), and proposed ROM/SG for $\tau = 1$ (—▲—), $\tau = 10$ (—▲—), $\tau = 100$ (—▲—), $\tau = \infty$ (—▲—)

Leveraging inexactness to accelerate PDE-constrained optimization

- Framework introduced for accelerating **deterministic** and **stochastic** PDE-constrained optimization problems
  - Adaptive *model reduction*
  - *Partially converged* primal and adjoint solutions
  - Dimension-adaptive *sparse grids*
- Inexactness **managed** with flexible **trust region** method
- Applied to variety of problems in computational mechanics and outperforms state-of-the-art methods
  - **1.6**× speedup on (deterministic) shape design of aircraft
  - **100**× speedup on (stochastic) optimal control of 1D flow

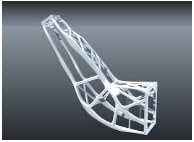


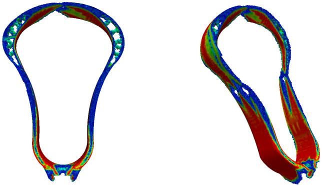


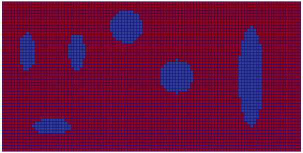


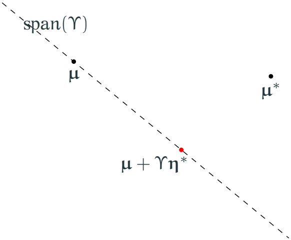
Extension to problems with many parameters

- Topology optimization[3] and inverse problems
- **Nested reduction** of state and parameter
- Multifidelity trust region method to globalize **state** reduction
- Linesearch/subspace method to globalize **parameter** reduction



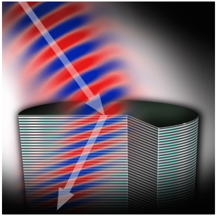


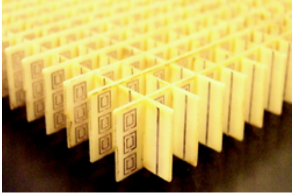




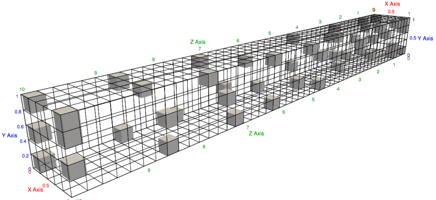
[3] Increasingly relevant due to emergence of Additive Manufacturing – ***MIT Technology Review***, **Top 10 Technological Breakthrough 2013**

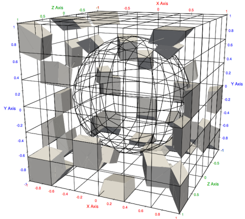
Extension to multiscale problems





- **Existing multiscale methods** are extremely expensive
  - Single simulation: 203 hours (≈ 8.5 days), 41760 cores [Knap et. al., 2016]
  - Not amenable to optimization (many-query)
- **Hyperreduced models** at each scale [Zahr et al., 2016a] – embedded in trust region optimization framework to *design microstructure* to achieve *macroscale objectives*





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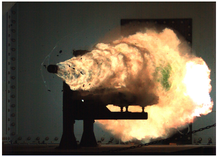

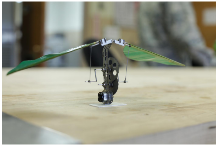

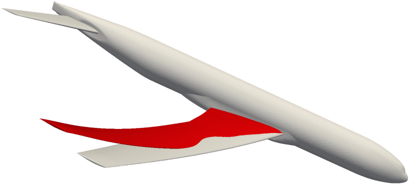

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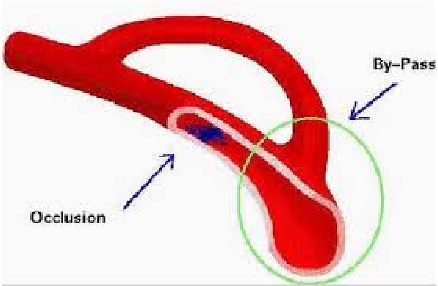
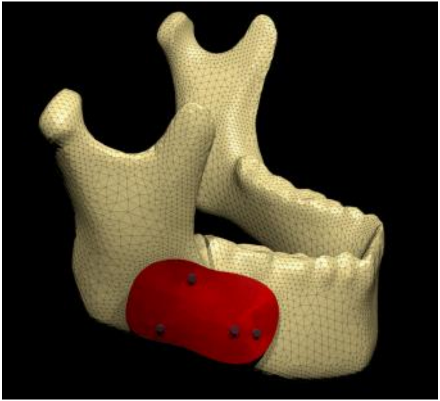
PDE optimization is ubiquitous in science and engineering

Design: Find system that optimizes performance metric, satisfies constraints





Shape design of arterial bypass (left) and shape/topology design of patient-specific implant (right)

Overview of global convergence theory[4]

Let $\{\mu_k\}$ be a sequence of iterates produced by the algorithm and suppose there exists $\epsilon > 0$ such that $\|\nabla m_k(\mu_k)\| > 0$

Lemma 1: $\Delta_k \to 0$

- Fraction of Cauchy decrease
- $|F(\mu_k) - F(\hat{\mu}_k) + \psi_k(\hat{\mu}_k) - \psi_k(\mu_k)| \leq \sigma\,[\eta \min\{m_k(\mu_k) - m_k(\hat{\mu}_k),\, r_k\}]^{1/\omega}$

Lemma 2: $\rho_k \to 1$

- Fraction of Cauchy decrease
- $|F(\mu_k) - F(\hat{\mu}_k) + m_k(\hat{\mu}_k) - m_k(\mu_k)| \leq \zeta\Delta_k$

Theorem 1: $\liminf \|\nabla F(\mu_k)\| = 0$

- Contradiction from Lemma 1 and 2 $\implies$ $\liminf \|\nabla m_k(\mu_k)\| = 0$
- $\|\nabla F(\mu_k) - \nabla m_k(\mu_k)\| \leq \xi \min\{\|\nabla m_k(\mu)\|,\, \Delta_k\}$

[4] Closely parallels convergence theory in [Moré, 1983, Kouri et al., 2014]

Definition of $\frac{\partial \mathbf{u}_r}{\partial \boldsymbol{\mu}}$: minimum-residual reduced sensitivities

Traditional sensitivity analysis ($\boldsymbol{\Theta} = \mathbf{I}$)

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

+ Guaranteed to produce *exact* derivatives of ROM quantities of interest
– Requires 2nd derivatives of $\mathbf{r}$
– $\boldsymbol{\Phi} \frac{\partial \mathbf{u}_r}{\partial \boldsymbol{\mu}}$ not guaranteed to be good approximate of $\frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}}$

Definition of $\frac{\partial \mathbf{u}_r}{\partial \mu}$: minimum-residual reduced sensitivities

Minimum-residual sensitivity analysis

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

+ **Minimum-residual property** – optimality, monotonicity, interpolation
+ Does not require 2nd derivatives of $\mathbf{r}$
– $\widehat{\frac{\partial \mathbf{u}_r}{\partial \mu}} \neq \frac{\partial \mathbf{u}_r}{\partial \mu}$, i.e., it is not the exact sensitivity[5]

[5] These quantities agree if $\boldsymbol{\Phi}^{\partial} = \boldsymbol{\Phi}$ and either $\boldsymbol{\Psi}$ is constant or the primal ROM is exact [Zahr et al., 2016b]

Hyperreduction to reduce complexity of nonlinear terms

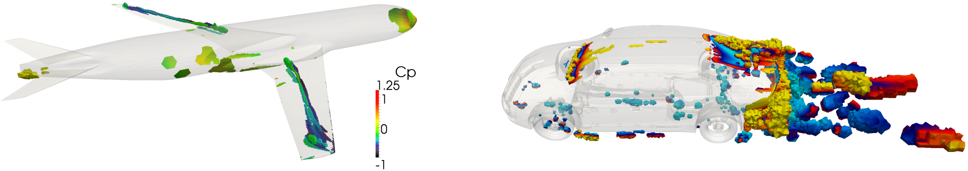
Despite **reduced dimensionality**, $\mathcal{O}(n_{\mathbf{u}})$ operations are required to evaluate

$$\boldsymbol{\Psi}^T \mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r, \boldsymbol{\mu}) \qquad \boldsymbol{\Psi}^T \frac{\partial \mathbf{r}}{\partial \mathbf{u}}(\boldsymbol{\Phi}\mathbf{u}_r, \boldsymbol{\mu})\boldsymbol{\Phi}$$

Solution: only perform minimization over a *subset* of the spatial domain

$$\underset{\mathbf{u}_r \in \mathbb{R}^{k_{\mathbf{u}}}}{\text{minimize}} \quad \|\mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r, \boldsymbol{\mu})\|_{\boldsymbol{\Theta}} \implies \underset{\mathbf{u}_r \in \mathbb{R}^{k_{\mathbf{u}}}}{\text{minimize}} \quad \left\|\mathbf{P}^T \mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r, \boldsymbol{\mu})\right\|_{\boldsymbol{\Theta}}$$

and **hyperreduced** model[6] is independent of $n_{\mathbf{u}}$



Sample mesh for CRM (left) and Passat (right) [Washabaugh, 2016]

[6] Masked minimum-residual property and weaker definitions of optimality, monotonicity, and interpolation hold

Proposed approach: managed inexactness

Replace expensive PDE with inexpensive approximation model

- **Reduced-order models** used for *inexact PDE evaluations*
- **Partially converged solutions** used for *inexact PDE evaluations*
- **Anisotropic sparse grids** used for *inexact integration* of risk measures

$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad F(\mu) \qquad \longrightarrow \qquad \underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad m_k(\mu)$$

Manage inexactness with trust region method

- Embedded in globally convergent **trust region** method
- **Error indicators** to account for *all* sources of inexactness
- **Refinement** of approximation model using *greedy algorithms*

$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad F(\mu) \qquad \longrightarrow \qquad \begin{array}{ll} \underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} & m_k(\mu) \\ \text{subject to} & \|\mu - \mu_k\| \leq \Delta_k \end{array}$$

Source of inexactness: Partially Converged Solution (PCS)

A τ-partially converged primal solution $\mathbf{u}^{\tau}(\boldsymbol{\mu})$ is any $\mathbf{u}$ satisfying

$$\|\mathbf{r}(\mathbf{u}, \boldsymbol{\mu})\|_{\boldsymbol{\Theta}} \leq \tau$$

A τ_1-τ_2-partially converged adjoint solution $\boldsymbol{\lambda}^{\tau_1, \tau_2}(\boldsymbol{\mu})$ is any $\boldsymbol{\lambda}$ satisfying

$$\left\|\mathbf{r}^{\boldsymbol{\lambda}}(\mathbf{u}^{\tau_1}(\boldsymbol{\mu}), \boldsymbol{\lambda}, \boldsymbol{\mu})\right\|_{\boldsymbol{\Theta}^{\lambda}} \leq \tau_2$$

Trust region method: ROM/PCS approximation model

Approximation models based on ROMs and partially converged solutions

$$m_k(\mu) = \mathcal{J}(\Phi_k u_r(\mu), \mu) \qquad \psi_k(\mu) = \mathcal{J}(u^{\tau_k}(\mu), \mu)$$

Error indicators from residual-based error bounds

$$\vartheta_k(\mu) = \|r(\Phi_k u_r(\mu_k), \mu_k)\|_\Theta + \|r(\Phi_k u_r(\mu), \mu)\|_\Theta$$
$$\varphi_k(\mu) = \|r(\Phi_k u_r(\mu), \mu)\|_\Theta + \left\|r^\lambda(\Phi_k u_r(\mu), \Psi_k \lambda_r(\mu), \mu)\right\|_{\Theta^\lambda}$$
$$\theta_k(\mu) = \|r(u^{\tau_k}(\mu_k), \mu_k)\|_\Theta + \|r(u^{\tau_k}(\mu), \mu)\|_\Theta$$

Adaptivity to refine basis at trust region center

$$\Phi_k = \begin{bmatrix} u^{\alpha_k}(\mu_k) & \lambda^{\alpha_k, \beta_k}(\mu_k) & \mathtt{POD}(U_k) & \mathtt{POD}(V_k) \end{bmatrix}$$

$$U_k = \begin{bmatrix} u^{\alpha_0}(\mu_0) & \cdots & u^{\alpha_{k-1}}(\mu_{k-1}) \end{bmatrix} \qquad V_k = \begin{bmatrix} \lambda^{\alpha_0, \beta_0}(\mu_0) & \cdots & \lambda^{\alpha_{k-1}, \beta_{k-1}}(\mu_{k-1}) \end{bmatrix}$$

and α_k, β_k, τ_k selected such that

$$\vartheta_k(\mu_k) \leq \kappa_\vartheta \Delta_k \qquad \varphi_k(\mu_k) \leq \kappa_\varphi \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$$
$$\theta_k^\omega(\hat{\mu}_k) \leq \eta \min\{m_k(\mu_k) - m_k(\hat{\mu}_k), r_k\}$$

Trust region method: ROM/PCS approximation model

Approximation models based on ROMs and partially converged solutions

$$m_k(\mu) = \mathcal{J}(\Phi_k \mathbf{u}_r(\mu), \mu) \qquad \psi_k(\mu) = \mathcal{J}(\mathbf{u}^{\tau_k}(\mu), \mu)$$

Error indicators from residual-based error bounds

$$\vartheta_k(\mu) = ||\mathbf{r}(\Phi_k \mathbf{u}_r(\mu_k), \mu_k)||_{\Theta} + ||\mathbf{r}(\Phi_k \mathbf{u}_r(\mu), \mu)||_{\Theta}$$

$$\varphi_k(\mu) = ||\mathbf{r}(\Phi_k \mathbf{u}_r(\mu), \mu)||_{\Theta} + \left|\left|\mathbf{r}^{\lambda}(\Phi_k \mathbf{u}_r(\mu), \Psi_k \lambda_r(\mu), \mu)\right|\right|_{\Theta^{\lambda}}$$

$$\theta_k(\mu) = ||\mathbf{r}(\mathbf{u}^{\tau_k}(\mu_k), \mu_k)||_{\Theta} + ||\mathbf{r}(\mathbf{u}^{\tau_k}(\mu), \mu)||_{\Theta}$$

Adaptivity to refine basis at trust region center

$$\Phi_k = \begin{bmatrix} \mathbf{u}^{\alpha_k}(\mu_k) & \lambda^{\alpha_k, \beta_k}(\mu_k) & \mathtt{POD}(\mathbf{U}_k) & \mathtt{POD}(\mathbf{V}_k) \end{bmatrix}$$

$$\mathbf{U}_k = \begin{bmatrix} \mathbf{u}^{\alpha_0}(\mu_0) & \cdots & \mathbf{u}^{\alpha_{k-1}}(\mu_{k-1}) \end{bmatrix} \qquad \mathbf{V}_k = \begin{bmatrix} \lambda^{\alpha_0, \beta_0}(\mu_0) & \cdots & \lambda^{\alpha_{k-1}, \beta_{k-1}}(\mu_{k-1}) \end{bmatrix}$$

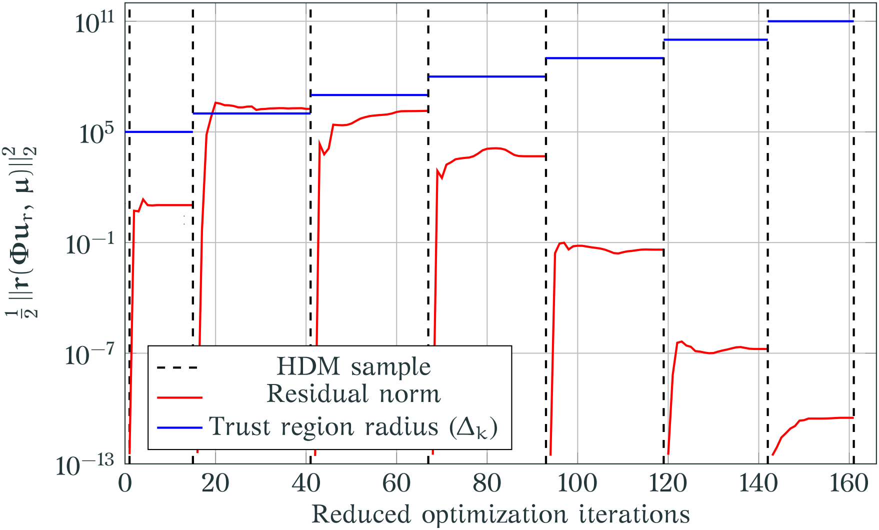
and α_k, β_k, τ_k selected such that

$$\vartheta_k(\mu_k) \leq \kappa_{\vartheta} \Delta_k \qquad \varphi_k(\mu_k) \leq \kappa_{\varphi} \min\{||\nabla m_k(\mu_k)||, \Delta_k\}$$

$$\theta_k^{\omega}(\hat{\mu}_k) \leq \eta \min\{m_k(\mu_k) - m_k(\hat{\mu}_k), r_k\}$$

$$\liminf_{k \to \infty} ||\nabla \mathcal{J}(\mathbf{u}(\mu_k), \mu_k)|| = 0$$

Error-aware trust region behavior



Source of inexactness: anisotropic sparse grids

1D Quadrature Rules: Define the difference operator

$$\Delta_k^j \equiv \mathbb{E}_k^j - \mathbb{E}_k^{j-1}$$

where $\mathbb{E}_k^0 \equiv 0$ and $\mathbb{E}_k^j$ as the level-j 1d quadrature rule for dimension k

Anisotropic Sparse Grid: Define the index set $\mathcal{I} \subset \mathbb{N}^{n_\xi}$ and

$$\mathbb{E}_{\mathcal{I}} \equiv \sum_{\mathbf{i} \in \mathcal{I}} \Delta_1^{i_1} \otimes \cdots \otimes \Delta_{n_\xi}^{i_{n_\xi}}$$

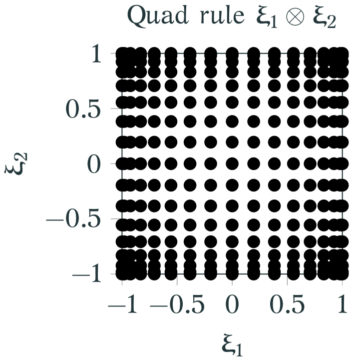
Neighbors: Let $\mathcal{I}^c = \mathbb{N}^{n_\xi} \setminus \mathcal{I}$

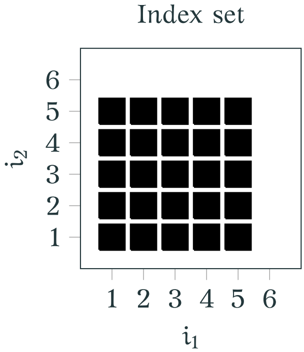
$$\mathcal{N}(\mathcal{I}) = \{\mathbf{i} \in \mathcal{I}^c \mid \mathbf{i} - \mathbf{e}_j \in \mathcal{I},\, j = 1, \ldots, n_\xi\}$$

Truncation Error: [Gerstner and Griebel, 2003, Kouri et al., 2013]

$$\mathbb{E} - \mathbb{E}_{\mathcal{I}} = \sum_{\mathbf{i} \in \mathcal{I}^c} \Delta_1^{i_1} \otimes \cdots \otimes \Delta_{n_\xi}^{i_{n_\xi}} \approx \sum_{\mathbf{i} \in \mathcal{N}(\mathcal{I})} \Delta_1^{i_1} \otimes \cdots \otimes \Delta_{n_\xi}^{i_{n_\xi}} = \mathbb{E}_{\mathcal{N}(\mathcal{I})}$$

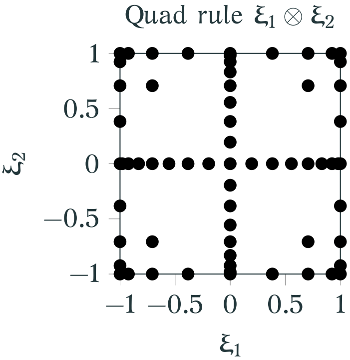
Tensor product quadrature

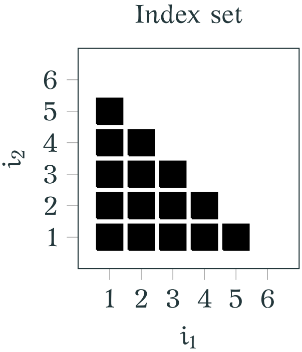




Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

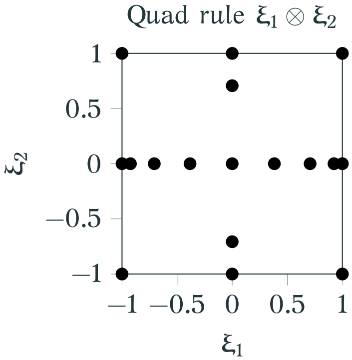
Isotropic sparse grid quadrature

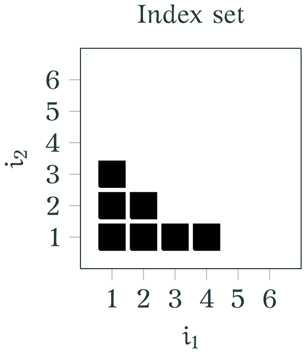




Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

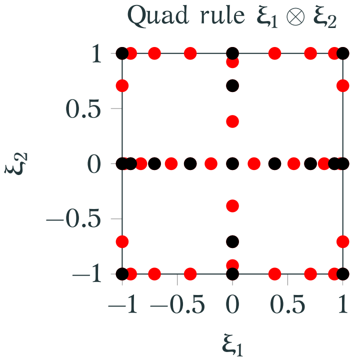
Anisotropic sparse grid quadrature

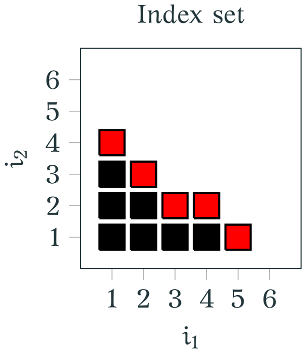




Index set ($\mathcal{I}$) – ● Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

Anisotropic sparse grid quadrature: neighbors





Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

Derivation of gradient error indicator

For brevity, let

$$\mathcal{J}(\boldsymbol{\xi}) \leftarrow \mathcal{J}(\mathbf{u}(\boldsymbol{\mu},\boldsymbol{\xi}),\boldsymbol{\mu},\boldsymbol{\xi})$$

$$\nabla\mathcal{J}(\boldsymbol{\xi}) \leftarrow \nabla\mathcal{J}(\mathbf{u}(\boldsymbol{\mu},\boldsymbol{\xi}),\boldsymbol{\mu},\boldsymbol{\xi})$$

$$\mathcal{J}_r(\boldsymbol{\xi}) = \mathcal{J}(\boldsymbol{\Phi}\mathbf{u}_r(\boldsymbol{\mu},\boldsymbol{\xi}),\boldsymbol{\mu},\boldsymbol{\xi})$$

$$\nabla\mathcal{J}_r(\boldsymbol{\xi}) = \nabla\mathcal{J}(\boldsymbol{\Phi}\mathbf{u}_r(\boldsymbol{\mu},\boldsymbol{\xi}),\boldsymbol{\mu},\boldsymbol{\xi})$$

$$\mathbf{r}_r(\boldsymbol{\xi}) = \mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r(\boldsymbol{\mu},\boldsymbol{\xi}),\boldsymbol{\mu},\boldsymbol{\xi})$$

$$\mathbf{r}_r^{\boldsymbol{\lambda}}(\boldsymbol{\xi}) = \mathbf{r}^{\boldsymbol{\lambda}}(\boldsymbol{\Phi}\mathbf{u}_r(\boldsymbol{\mu},\boldsymbol{\xi}),\boldsymbol{\Psi}\boldsymbol{\lambda}_r(\boldsymbol{\mu},\boldsymbol{\xi}),\boldsymbol{\mu},\boldsymbol{\xi})$$

Separate total error into contributions from ROM inexactness and SG truncation

$$||\mathbb{E}[\nabla\mathcal{J}] - \mathbb{E}_{\mathcal{I}}[\nabla\mathcal{J}_r]|| \leq \mathbb{E}\left[||\nabla\mathcal{J} - \nabla\mathcal{J}_r||\right] + ||\mathbb{E}\left[\nabla\mathcal{J}_r\right] - \mathbb{E}_{\mathcal{I}}\left[\nabla\mathcal{J}_r\right]||$$

Derivation of gradient error indicator

For brevity, let

$$\begin{aligned}
\mathcal{J}(\xi) &\leftarrow \mathcal{J}(\mathbf{u}(\mu, \xi), \mu, \xi) \\
\nabla\mathcal{J}(\xi) &\leftarrow \nabla\mathcal{J}(\mathbf{u}(\mu, \xi), \mu, \xi) \\
\mathcal{J}_r(\xi) &= \mathcal{J}(\mathbf{\Phi u}_r(\mu, \xi), \mu, \xi) \\
\nabla\mathcal{J}_r(\xi) &= \nabla\mathcal{J}(\mathbf{\Phi u}_r(\mu, \xi), \mu, \xi) \\
\mathbf{r}_r(\xi) &= \mathbf{r}(\mathbf{\Phi u}_r(\mu, \xi), \mu, \xi) \\
\mathbf{r}_r^{\lambda}(\xi) &= \mathbf{r}^{\lambda}(\mathbf{\Phi u}_r(\mu, \xi), \mathbf{\Psi \lambda}_r(\mu, \xi), \mu, \xi)
\end{aligned}$$

Separate total error into contributions from ROM inexactness and SG truncation

$$\begin{aligned}
||\mathbb{E}[\nabla\mathcal{J}] - \mathbb{E}_{\mathcal{I}}[\nabla\mathcal{J}_r]|| &\leq \mathbb{E}\left[||\nabla\mathcal{J} - \nabla\mathcal{J}_r||\right] + ||\mathbb{E}\left[\nabla\mathcal{J}_r\right] - \mathbb{E}_{\mathcal{I}}\left[\nabla\mathcal{J}_r\right]|| \\
&\leq \zeta'\mathbb{E}\left[\alpha_1 \left|\left|\mathbf{r}\right|\right| + \alpha_2 \left|\left|\mathbf{r}^{\lambda}\right|\right|\right] + \mathbb{E}_{\mathcal{I}^c}\left[||\nabla\mathcal{J}_r||\right]
\end{aligned}$$

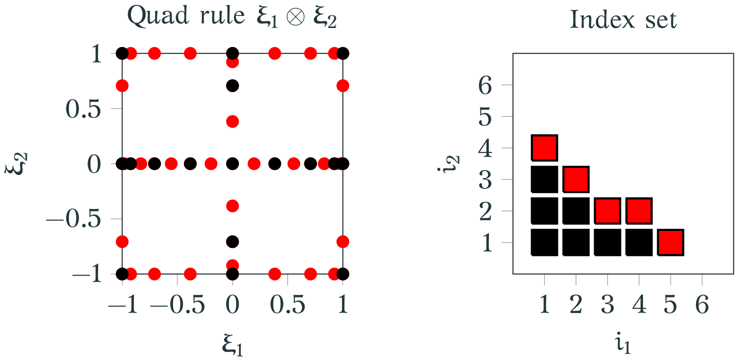
For brevity, let

$$\begin{aligned}
\mathcal{J}(\xi) &\leftarrow \mathcal{J}(\mathbf{u}(\mu, \xi), \mu, \xi) \\
\nabla\mathcal{J}(\xi) &\leftarrow \nabla\mathcal{J}(\mathbf{u}(\mu, \xi), \mu, \xi) \\
\mathcal{J}_r(\xi) &= \mathcal{J}(\boldsymbol{\Phi}\mathbf{u}_r(\mu, \xi), \mu, \xi) \\
\nabla\mathcal{J}_r(\xi) &= \nabla\mathcal{J}(\boldsymbol{\Phi}\mathbf{u}_r(\mu, \xi), \mu, \xi) \\
\mathbf{r}_r(\xi) &= \mathbf{r}(\boldsymbol{\Phi}\mathbf{u}_r(\mu, \xi), \mu, \xi) \\
\mathbf{r}_r^{\lambda}(\xi) &= \mathbf{r}^{\lambda}(\boldsymbol{\Phi}\mathbf{u}_r(\mu, \xi), \boldsymbol{\Psi}\boldsymbol{\lambda}_r(\mu, \xi), \mu, \xi)
\end{aligned}$$

Separate total error into contributions from ROM inexactness and SG truncation

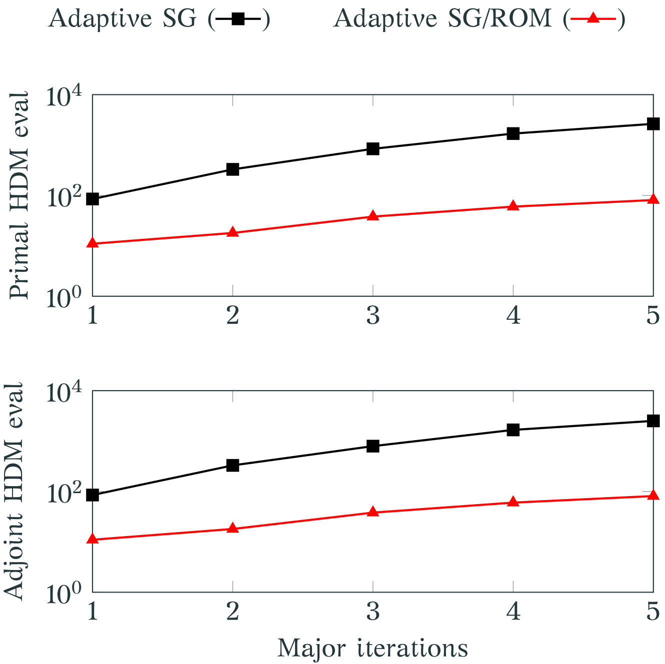
$$\begin{aligned}
||\mathbb{E}[\nabla\mathcal{J}] - \mathbb{E}_{\mathcal{I}}[\nabla\mathcal{J}_r]|| &\leq \mathbb{E}\left[||\nabla\mathcal{J} - \nabla\mathcal{J}_r||\right] + ||\mathbb{E}\left[\nabla\mathcal{J}_r\right] - \mathbb{E}_{\mathcal{I}}\left[\nabla\mathcal{J}_r\right]|| \\
&\leq \zeta'\mathbb{E}\left[\alpha_1\,||\mathbf{r}|| + \alpha_2\,\left|\left|\mathbf{r}^{\lambda}\right|\right|\right] + \mathbb{E}_{\mathcal{I}^c}\left[||\nabla\mathcal{J}_r||\right] \\
&\lesssim \zeta\left(\mathbb{E}_{\mathcal{I}\cup\mathcal{N}(\mathcal{I})}\left[\alpha_1\,||\mathbf{r}|| + \alpha_2\,\left|\left|\mathbf{r}^{\lambda}\right|\right|\right] + \alpha_3\mathbb{E}_{\mathcal{N}(\mathcal{I})}\left[||\nabla\mathcal{J}_r||\right]\right)
\end{aligned}$$

Adaptivity: Dimension-adaptive greedy method

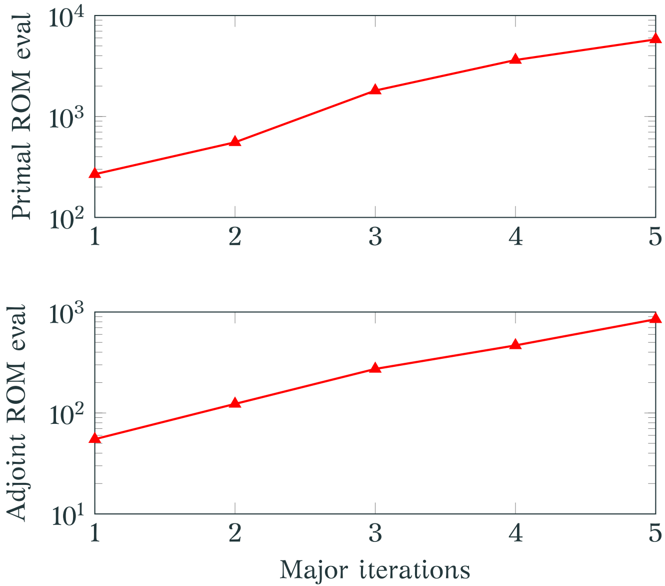


Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

Significant reduction in number of queries to HDM in comparison to state-of-the-art [Kouri et al., 2014]



At a price ... a large number of ROM evaluations



Extension to time-dependent problems

- **Applications**: inverse problems, optimal flapping flight and swimming[7] and design of helicopter blades, wind turbines, and turbomachinery
- Monolithic **space-time** formulation of reduced-order model
  - Increased speed due to natural **parallelism** in *space and time*
  - Treat as **steady state** problem in $n_{sd} + 1$ dimensions
- **Error indicators and adaptivity** algorithms in space-time setting to solve with multifidelity trust region method

Un-optimized flapping motion (left), optimal control (center), and optimal control and time-morphed geometry (right)

[7] Insight into bio-locomotion, design of micro-aerial vehicles