

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

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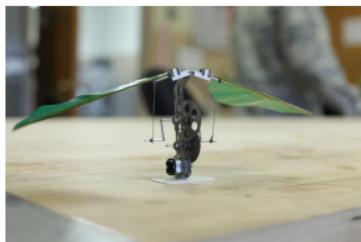


PDE optimization is ubiquitous in science and engineering

Design: Find system that optimizes performance metric, satisfies constraints



Aerodynamic shape design of automobile

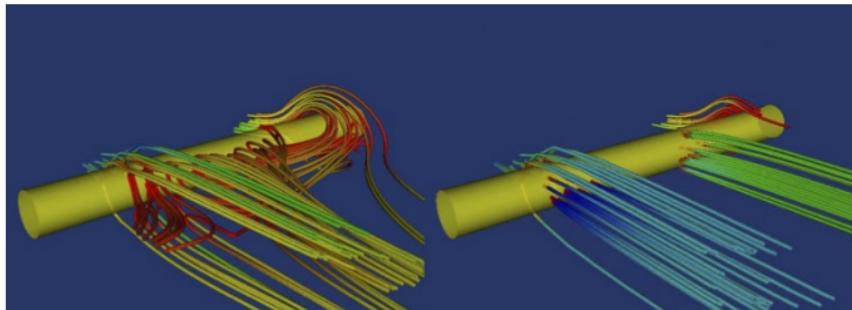


Optimal flapping motion of micro aerial vehicle

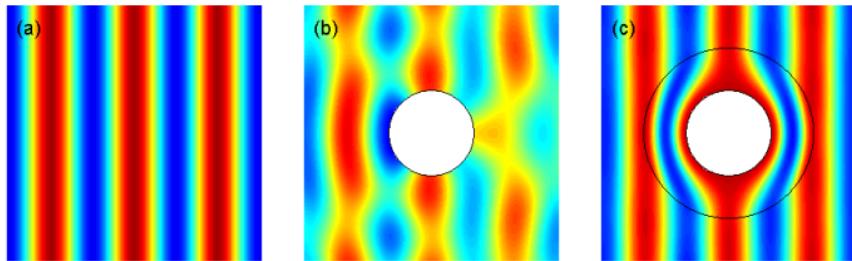


PDE optimization is ubiquitous in science and engineering

Control: Drive system to a desired state



Boundary flow control

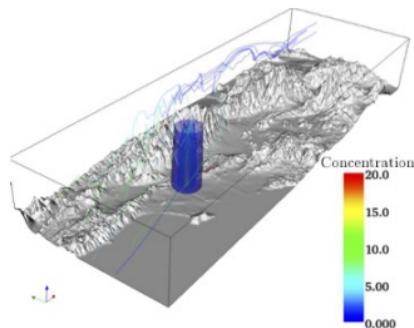
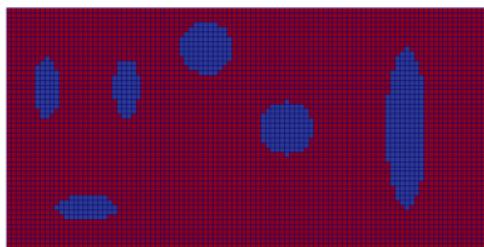


Metamaterial cloaking – electromagnetic invisibility

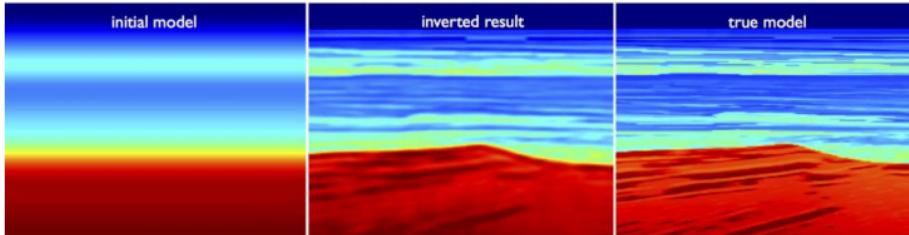


PDE optimization is ubiquitous in science and engineering

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

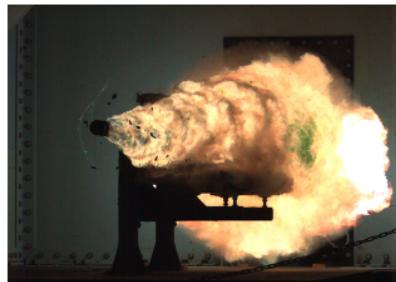


PDE optimization – a key player in next-gen problems

*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

$$\underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad \mathcal{J}(\boldsymbol{u}, \boldsymbol{\mu})$$

$$\text{subject to} \quad \mathbf{r}(\boldsymbol{u}; \boldsymbol{\mu}) = 0$$

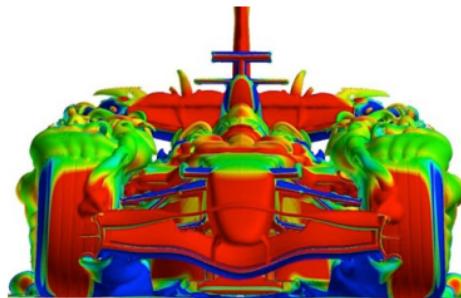
- $\mathbf{r} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \rightarrow \mathbb{R}^{n_u}$
- $\mathcal{J} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \rightarrow \mathbb{R}$
- $\boldsymbol{u} \in \mathbb{R}^{n_u}$
- $\boldsymbol{\mu} \in \mathbb{R}^{n_\mu}$

discretized PDE

quantity of interest

PDE state vector

optimization parameters



Nested approach to PDE-constrained optimization

Virtually all expense emanates from primal/dual PDE solves

Optimizer

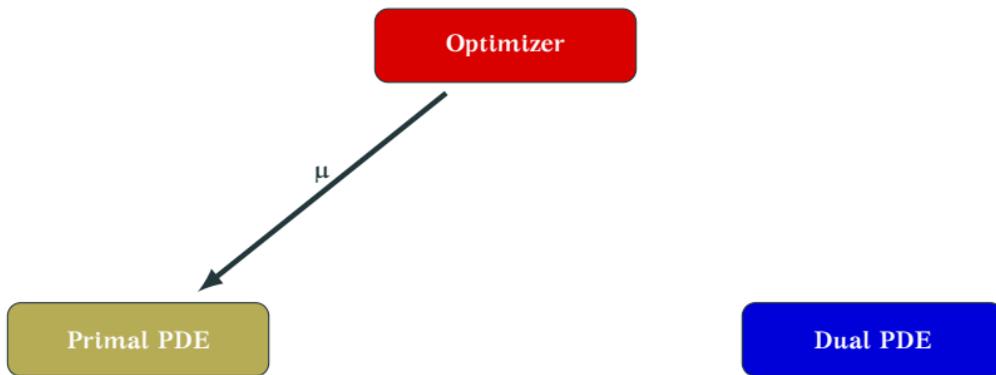
Primal PDE

Dual PDE



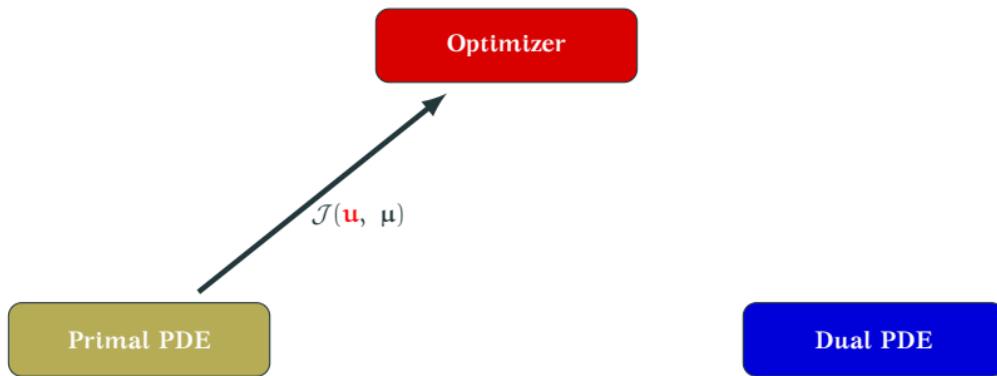
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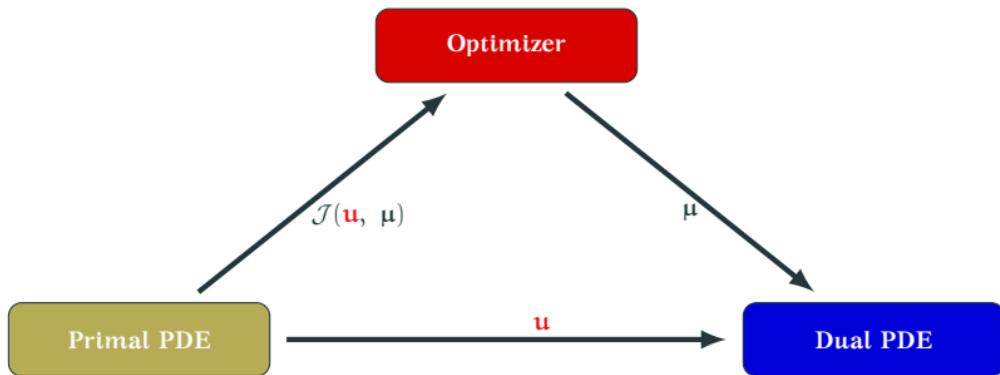
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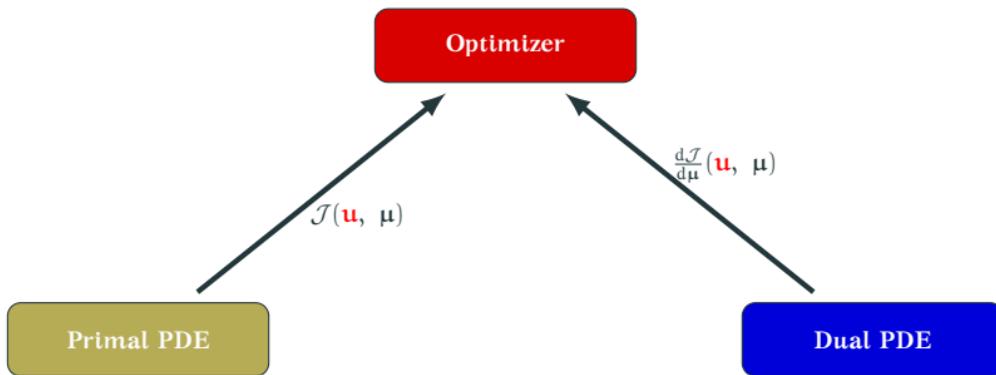
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Nested approach to PDE-constrained optimization

Virtually all expense emanates from primal/dual PDE solves



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

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

- $\mathbf{r} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \times \mathbb{R}^{n_\xi} \rightarrow \mathbb{R}^{n_u}$ discretized stochastic PDE
- $\mathcal{J} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \times \mathbb{R}^{n_\xi} \rightarrow \mathbb{R}$ 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
- $\mathbb{E}[\mathcal{F}] \equiv \int_{\Xi} \mathcal{F}(\boldsymbol{\xi}) \rho(\boldsymbol{\xi}) d\boldsymbol{\xi}$

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**

Optimizer

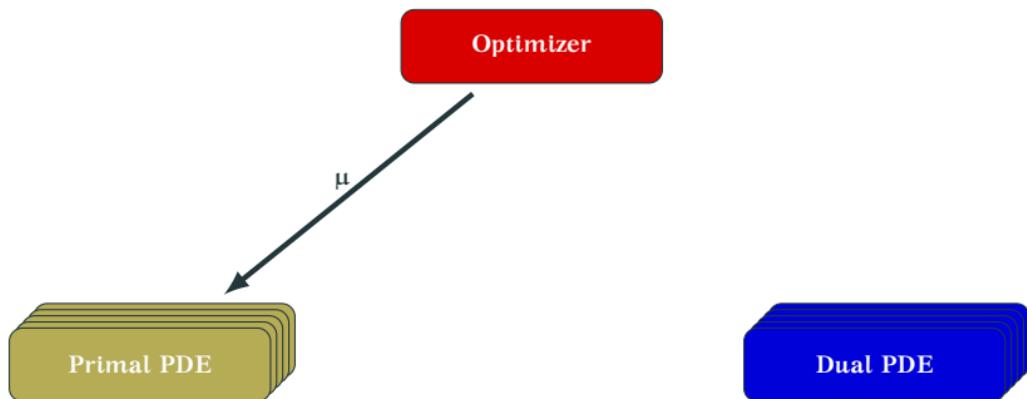
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Dual PDE



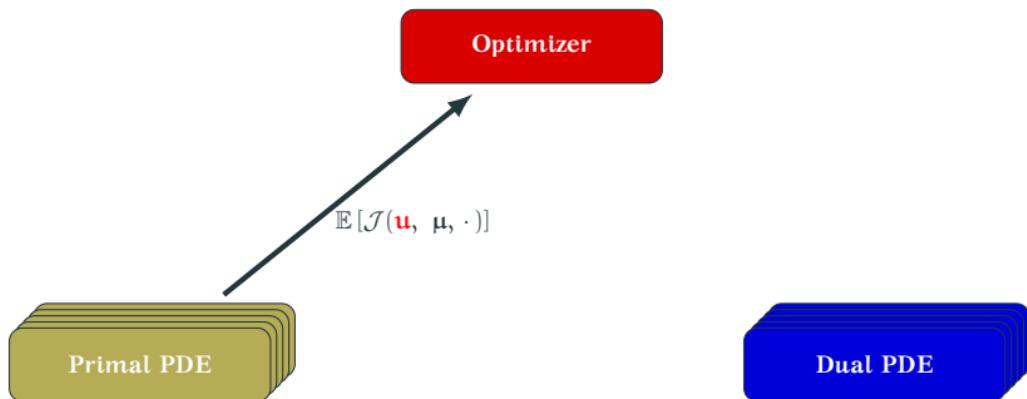
Nested approach to stochastic PDE-constrained optimization

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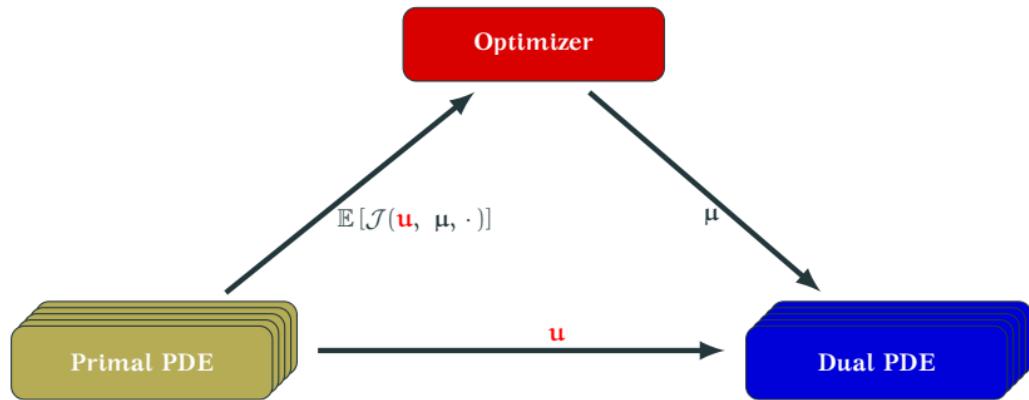
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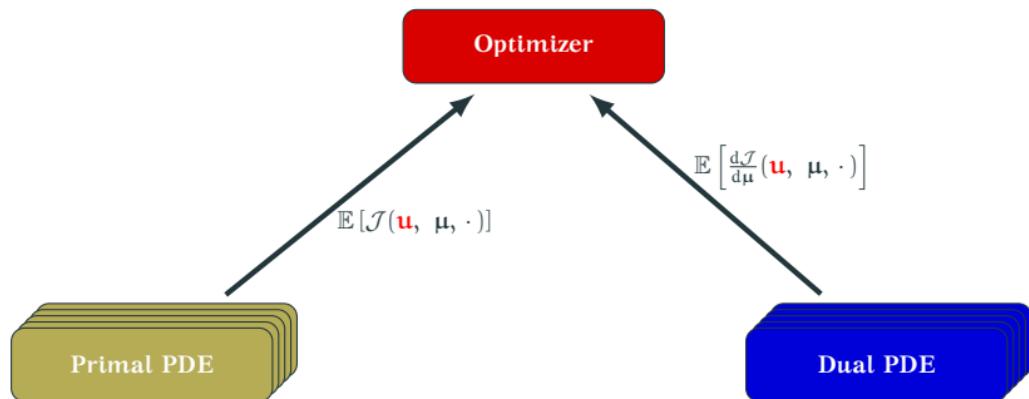
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Ensemble of primal/dual PDE solves increases cost by **orders of magnitude**



Nested approach to stochastic PDE-constrained optimization

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



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

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



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 indicators¹ to account for *all* sources of inexactness
- Refinement of approximation model using *greedy algorithms*

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



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

Relationship between the objective function and model

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

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

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



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

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

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

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

$$\hat{\mu}_k = \arg \min_{\mu \in \mathbb{R}^{n_\mu}} m_k(\mu) \text{ subject to } \|\mu - \mu_k\| \leq \Delta_k$$

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 $\rho_k \geq \eta_1$ **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** $\Delta_{k+1} \in (0, \gamma \|\hat{\mu}_k - \mu_k\|]$ **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 $\rho_k \geq \eta_2$ **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

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

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

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

- 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]

$$|F(\mu_k) - F(\mu) + m_k(\mu) - m_k(\mu_k)| \leq \zeta \vartheta_k(\mu) \quad \zeta > 0$$
$$\vartheta_k(\mu_k) \leq \kappa_\vartheta \Delta_k \quad \kappa_\vartheta \in (0, 1)$$

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

$$|F(\mu_k) - F(\mu) + \psi_k(\mu) - \psi_k(\mu_k)| \leq \sigma \theta_k(\mu) \quad \sigma > 0$$
$$\theta_k(\hat{\mu}_k)^\omega \leq \eta \min\{m_k(\mu_k) - m_k(\hat{\mu}_k), r_k\}$$
$$\omega, \eta \in (0, 1), r_k \rightarrow 0$$



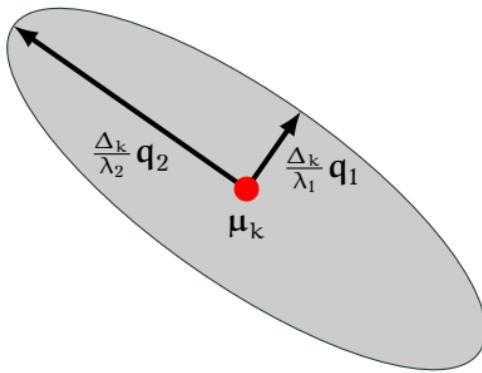
An interpretation of error-aware trust regions

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

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

Then, to first order²,

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



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

Assuming $\vartheta_k(\mu_k) = 0$, i.e., model exact at trust region center

A look at error-aware trust regions

Optimization of the Rosenbrock function

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

using the approximation models and error indicators

$$m_k(\boldsymbol{\mu}) \equiv G_k(\boldsymbol{\mu}; \epsilon_k, \delta_k)$$

$$\psi_k(\boldsymbol{\mu}) \equiv F(\boldsymbol{\mu})$$

$$\vartheta_k(\boldsymbol{\mu}) \equiv |F(\boldsymbol{\mu}) - G_k(\boldsymbol{\mu}; \epsilon_k, \delta_k)| + |F(\boldsymbol{\mu}_k) - G_k(\boldsymbol{\mu}_k; \epsilon_k, \delta_k)|$$

$$\varphi_k(\boldsymbol{\mu}) \equiv \|\nabla F(\boldsymbol{\mu}) - \nabla G_k(\boldsymbol{\mu}; \epsilon_k, \delta_k)\|$$

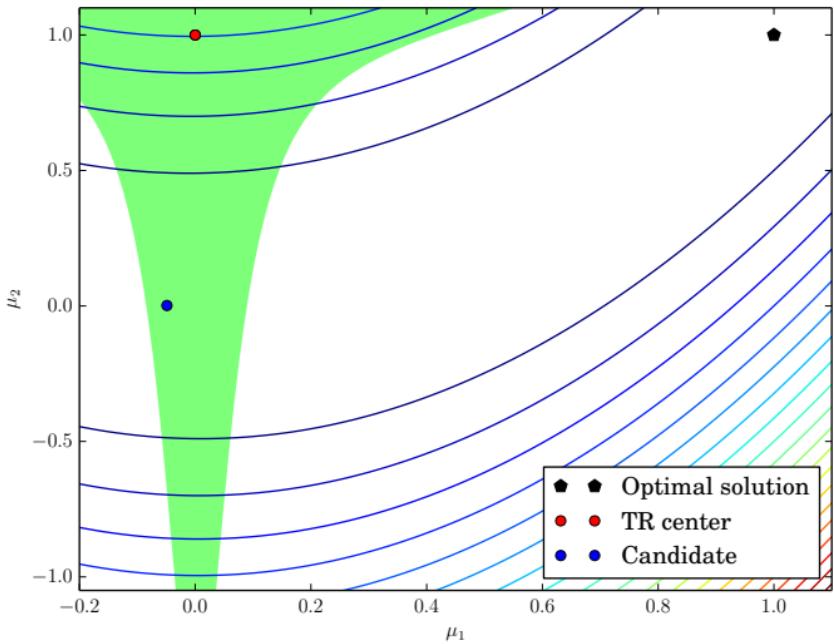
$$\theta_k(\boldsymbol{\mu}) \equiv 0$$

where $G_k(\boldsymbol{\mu}; \epsilon_k, \delta_k)$ is the inexact quadratic approximation of F at $\boldsymbol{\mu}_k$

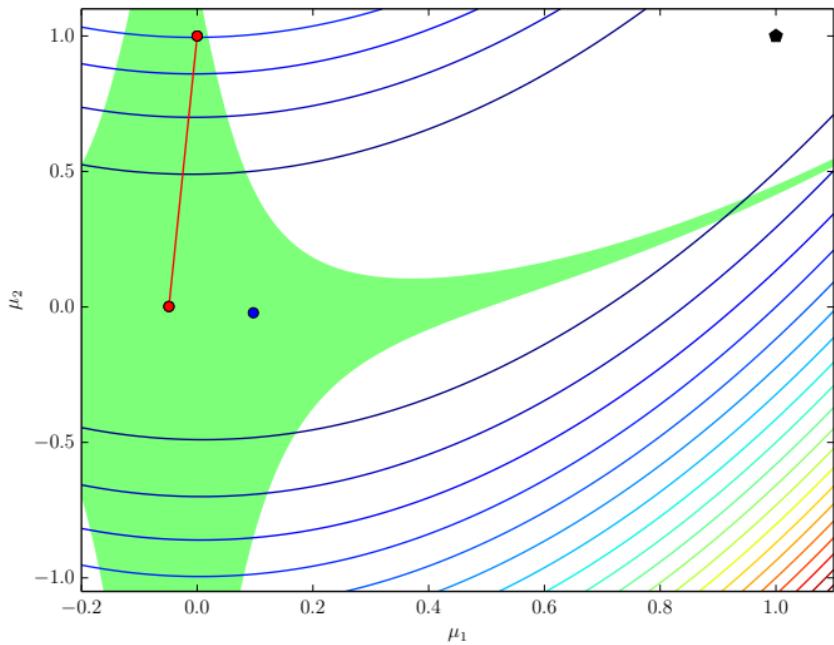
$$G_k(\boldsymbol{\mu}; \epsilon, \delta) \equiv F(\boldsymbol{\mu}_k) + \epsilon + (\nabla F(\boldsymbol{\mu}_k) + \delta \mathbf{1})^\top (\boldsymbol{\mu} - \boldsymbol{\mu}_k) + \frac{1}{2} (\boldsymbol{\mu} - \boldsymbol{\mu}_k)^\top \nabla^2 F(\boldsymbol{\mu}_k) (\boldsymbol{\mu} - \boldsymbol{\mu}_k)$$



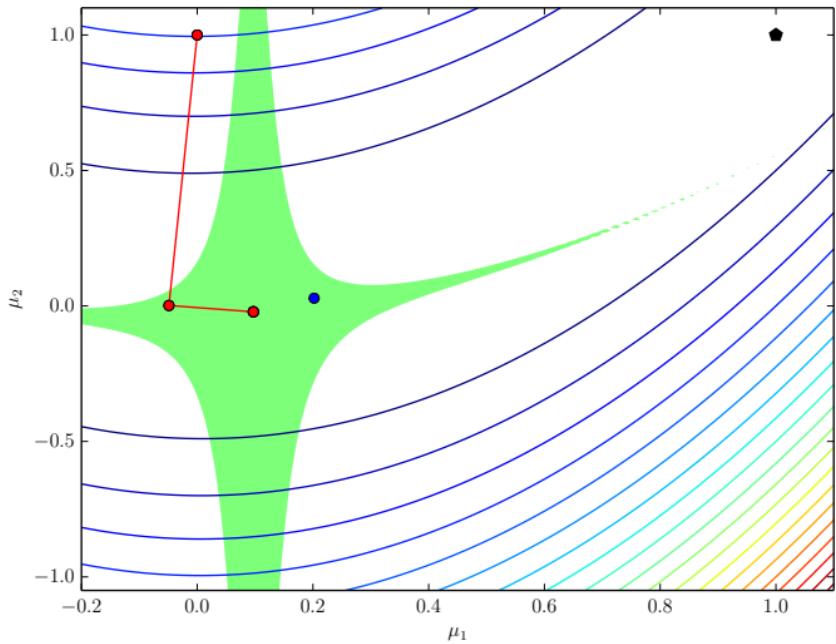
A look at error-aware trust regions



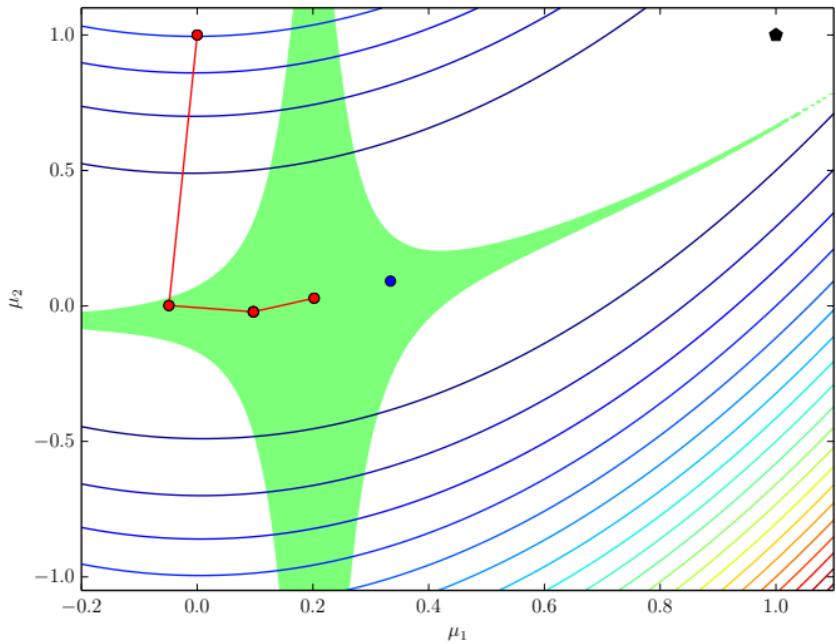
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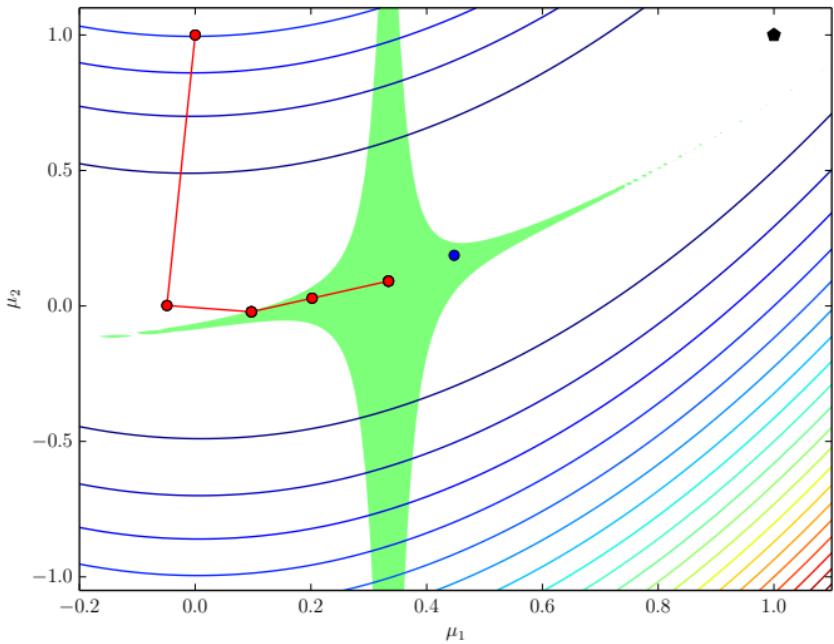
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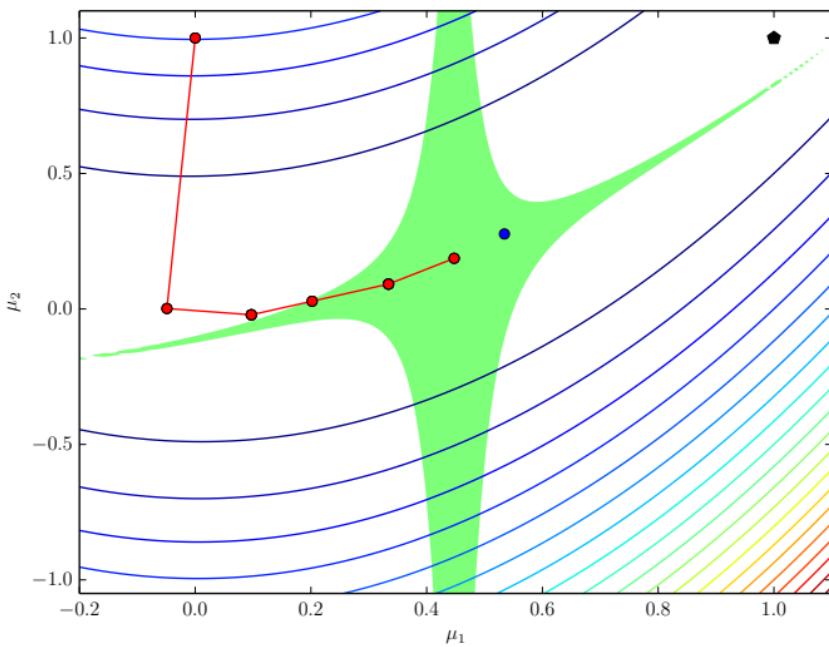
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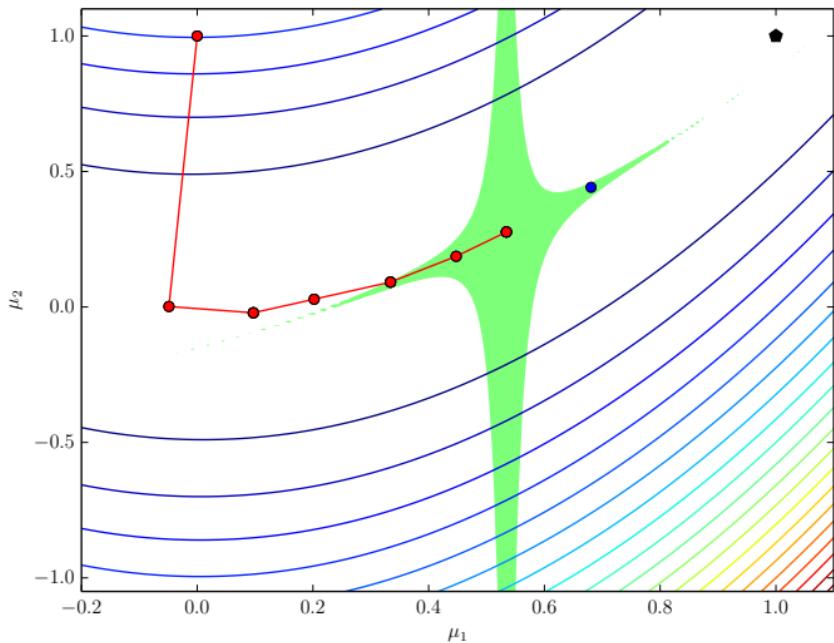
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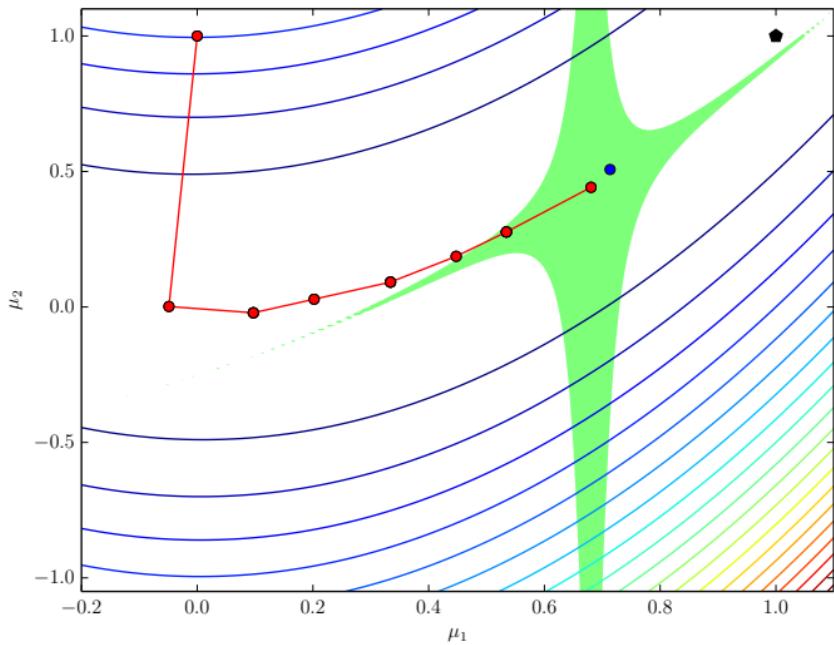
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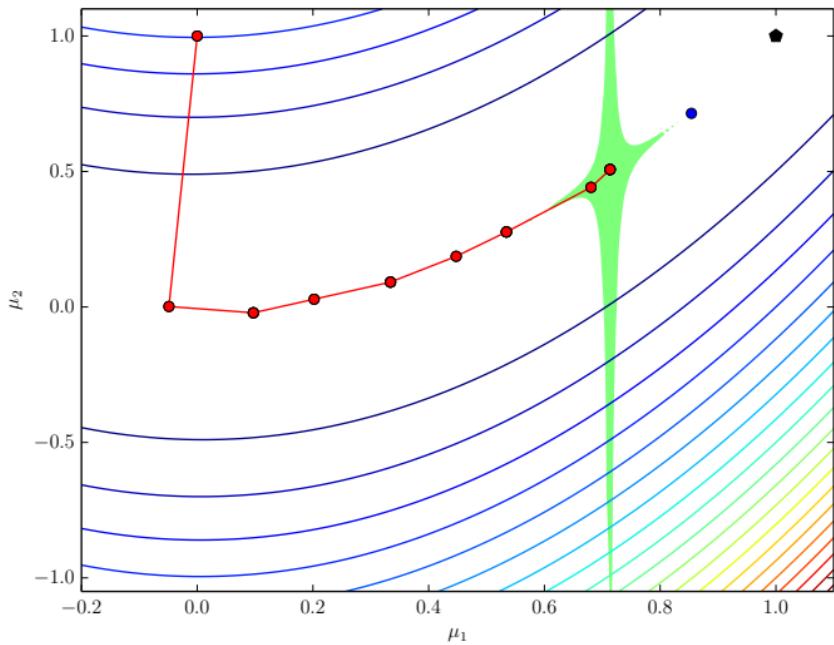
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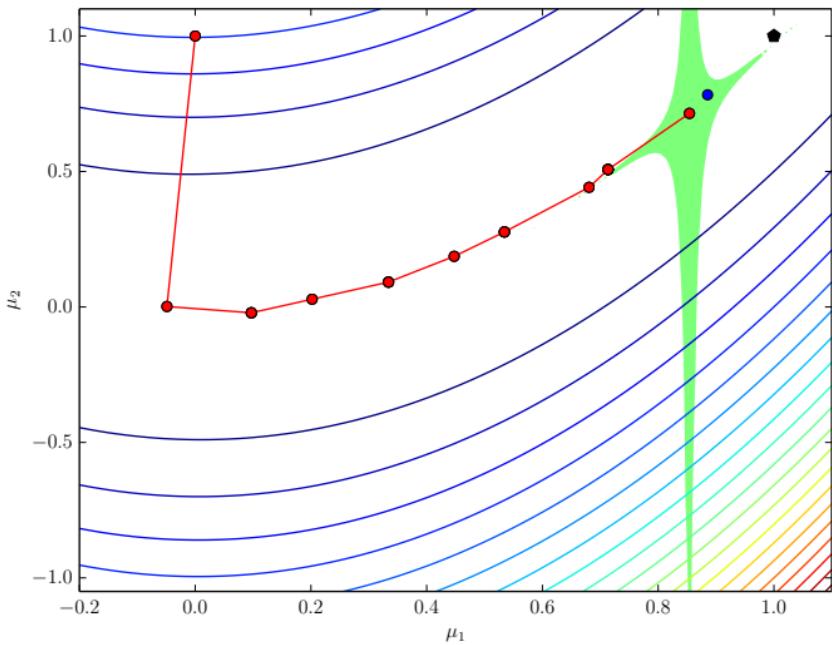
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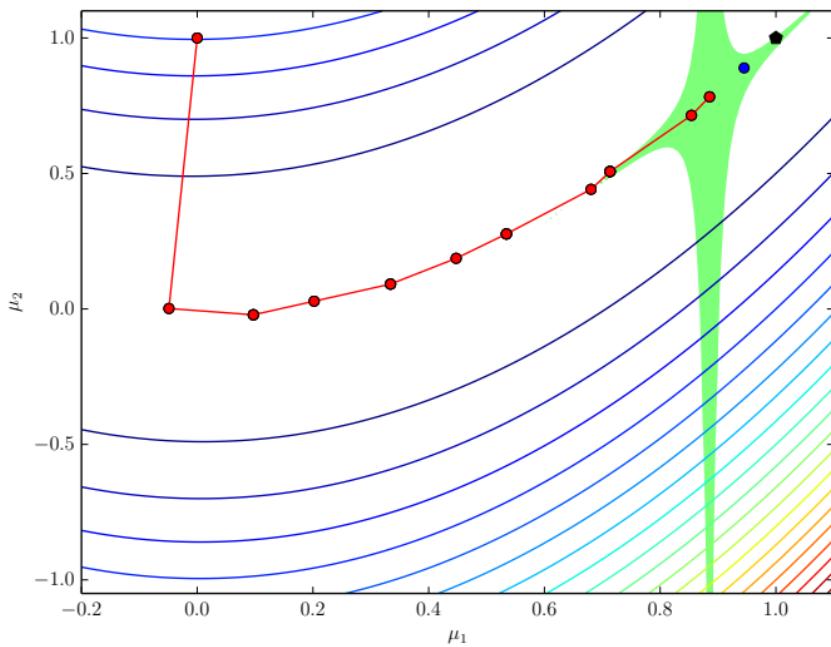
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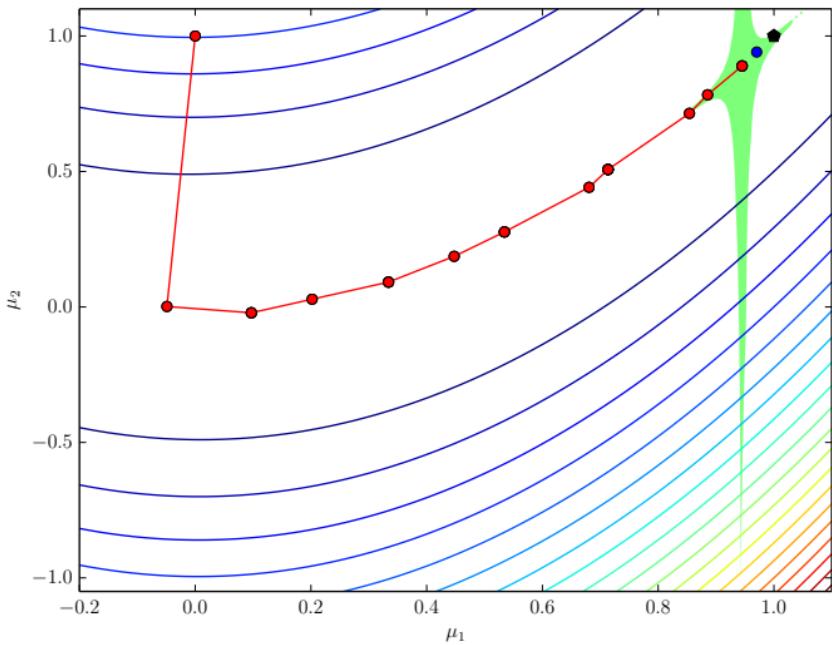
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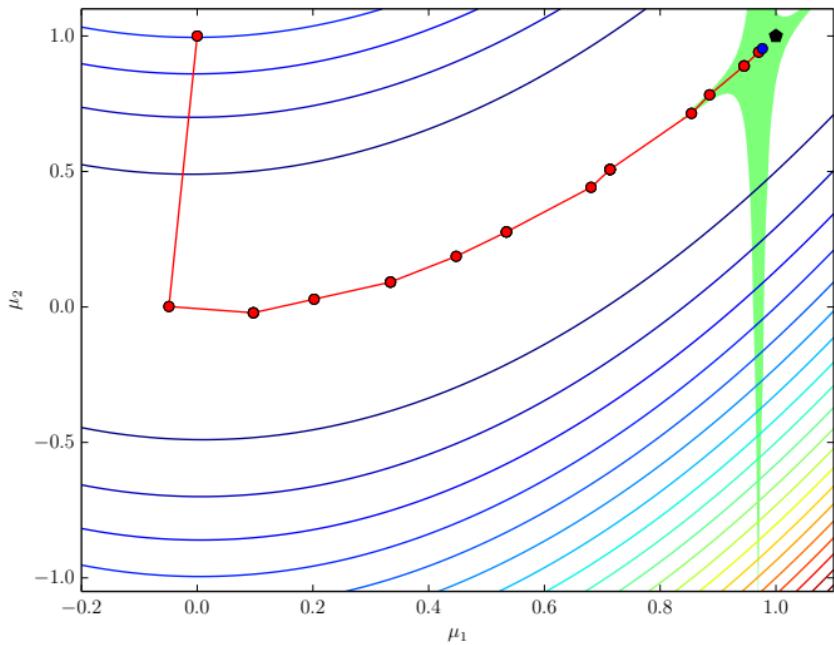
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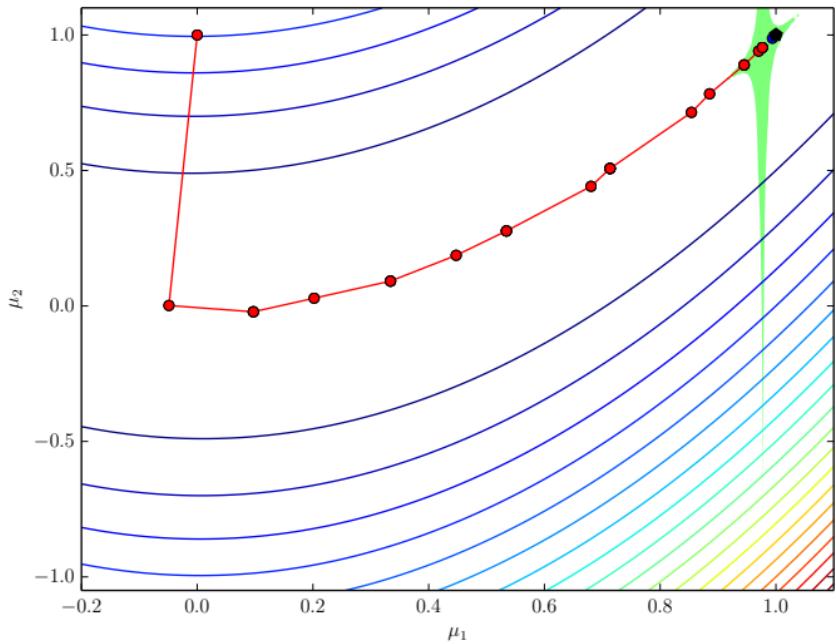
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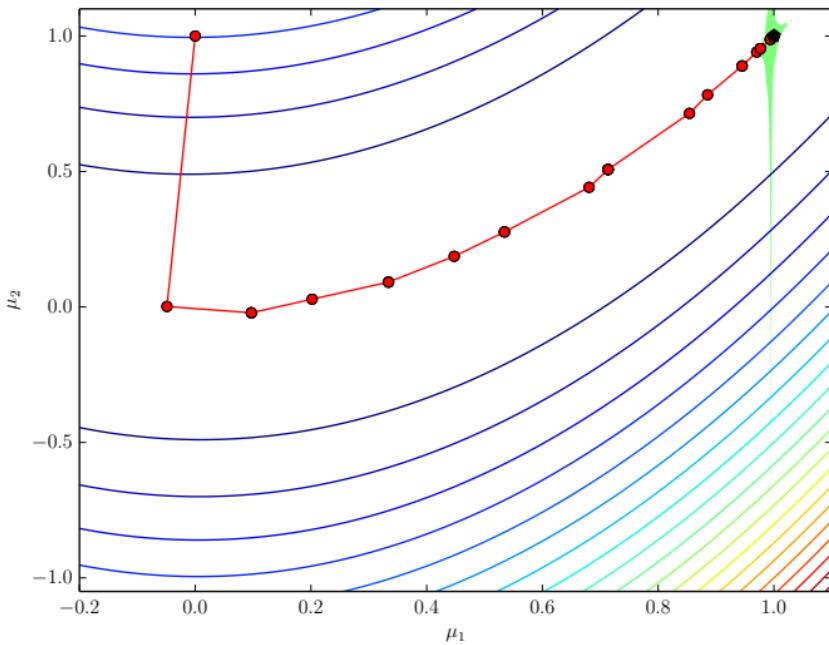
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A look at error-aware trust regions



A look at error-aware trust regions



Trust region ingredients for global convergence

Approximation models

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

Error indicators

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

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

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

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

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



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

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

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*

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

subject to $\|\mu - \mu_k\| \leq \Delta_k$



Source of inexactness: projection-based model reduction

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

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

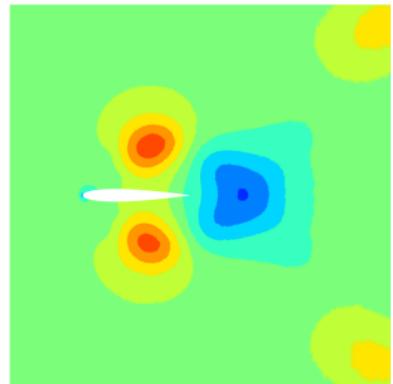
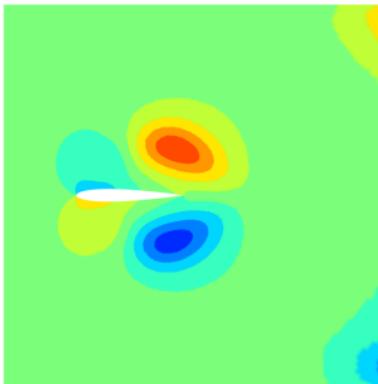
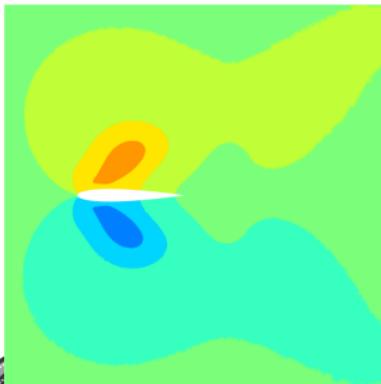
- $\Phi = [\Phi^1 \quad \dots \quad \Phi^{k_u}] \in \mathbb{R}^{n_u \times k_u}$ is the reduced (trial) basis ($n_u \gg k_u$)
- $\mathbf{u}_r \in \mathbb{R}^{k_u}$ are the reduced coordinates of \mathbf{u}
- Substitute into $\mathbf{r}(\mathbf{u}, \mu) = 0$ and project onto columnspace of a test basis $\Psi \in \mathbb{R}^{n_u \times k_u}$ to obtain a square system

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



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 Ψ : minimum-residual reduced-order models

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

$$\underset{u_r \in \mathbb{R}^{k_u}}{\text{minimize}} \quad \|r(\Phi u_r, \mu)\|_{\Theta} \quad \Theta \succ 0$$

which requires

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



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which requires

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

Implications of the minimum-residual property

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

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

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

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

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

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



Offline-online approach to optimization with ROMs



Schematic



μ -space



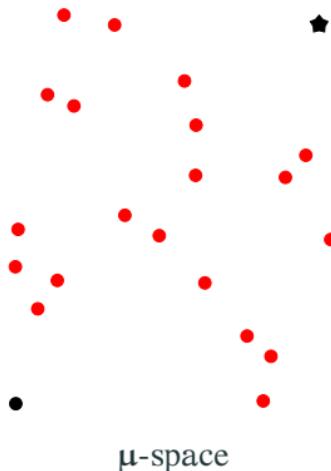
Breakdown of Computational Effort



Offline-online approach to optimization with ROMs



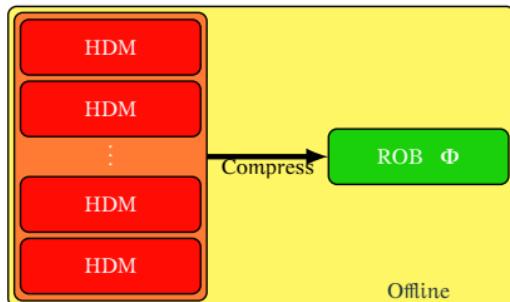
Schematic



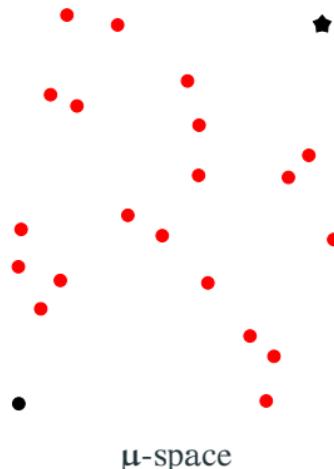
Breakdown of Computational Effort



Offline-online approach to optimization with ROMs



Schematic



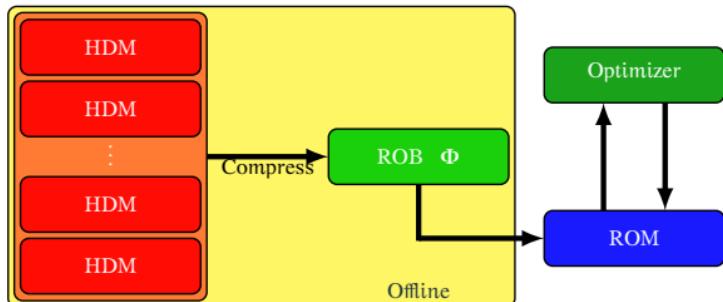
μ -space



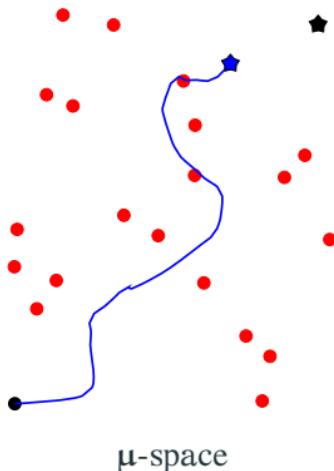
Breakdown of Computational Effort



Offline-online approach to optimization with ROMs



Schematic



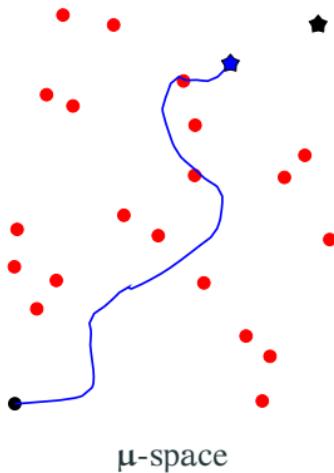
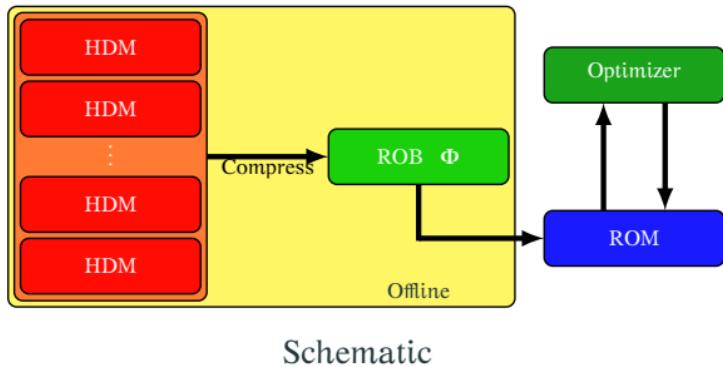
μ -space



Breakdown of Computational Effort



Offline-online approach to optimization with ROMs



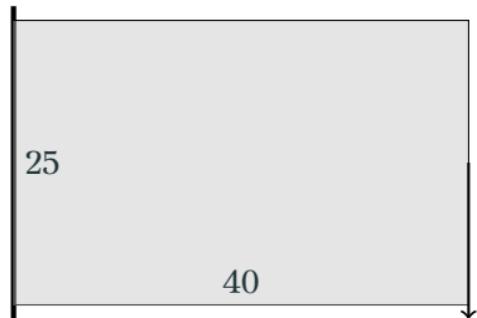
No convergence

Scales exponentially with N_μ

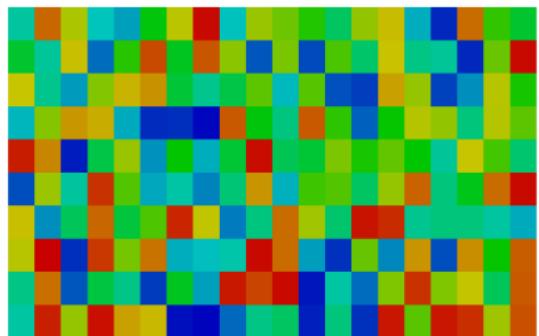


Numerical demonstration: offline-online breakdown

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



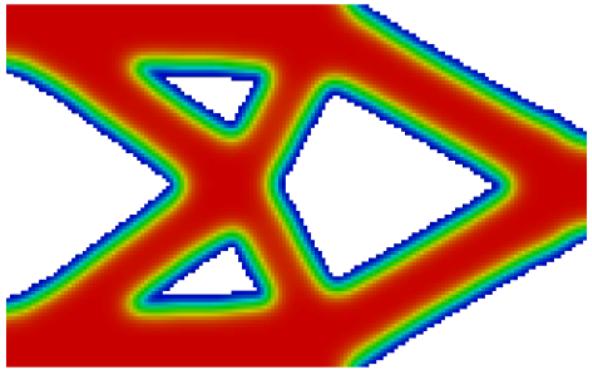
Stiffness maximization, volume constraint



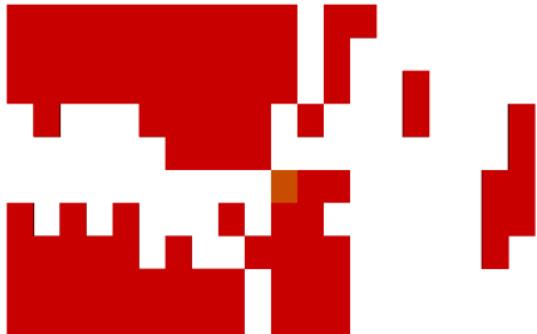
Parametrization with $n_\mu = 200$



Numerical demonstration: offline-online breakdown



Optimal Solution
 $(1.97 \times 10^4 \text{ s})$



ROM Solution

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



Trust region framework for optimization with ROMs



Schematic



μ -space

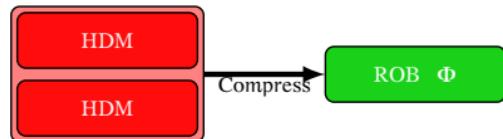


Breakdown of Computational Effort



BERKELEY LAB

Trust region framework for optimization with ROMs



Schematic



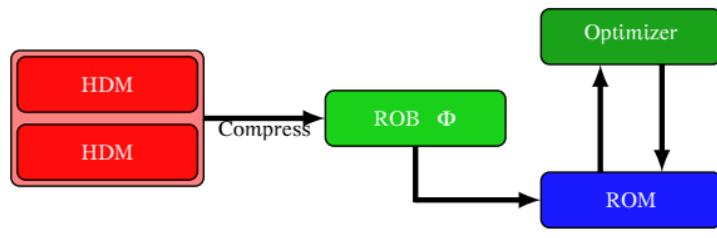
μ -space



Breakdown of Computational Effort



Trust region framework for optimization with ROMs



Schematic



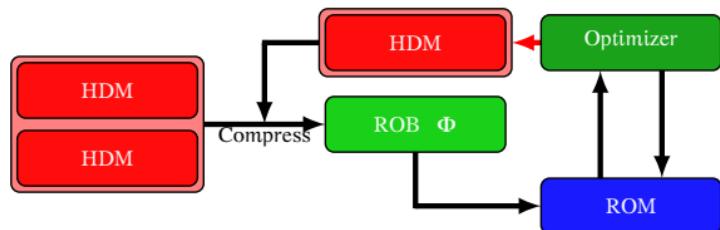
μ -space



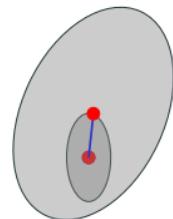
Breakdown of Computational Effort



Trust region framework for optimization with ROMs



Schematic



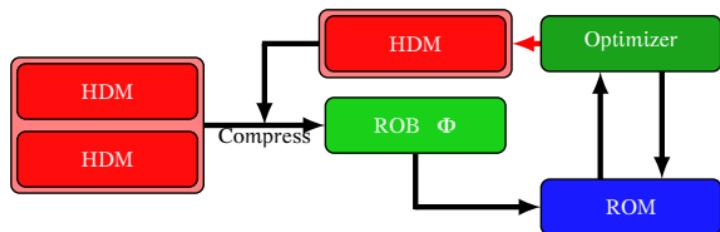
μ -space



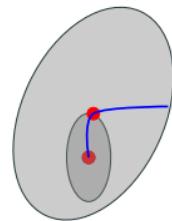
Breakdown of Computational Effort



Trust region framework for optimization with ROMs



Schematic



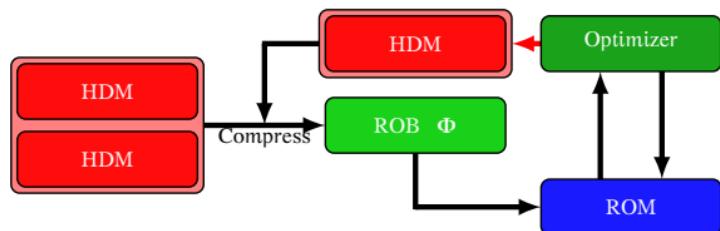
μ -space



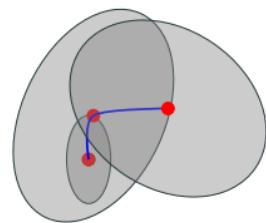
Breakdown of Computational Effort



Trust region framework for optimization with ROMs



Schematic



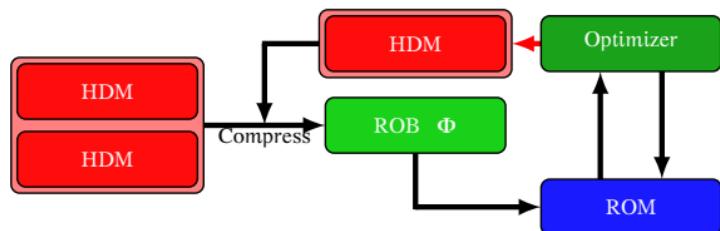
μ -space



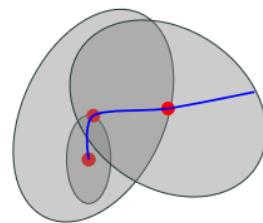
Breakdown of Computational Effort



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Schematic



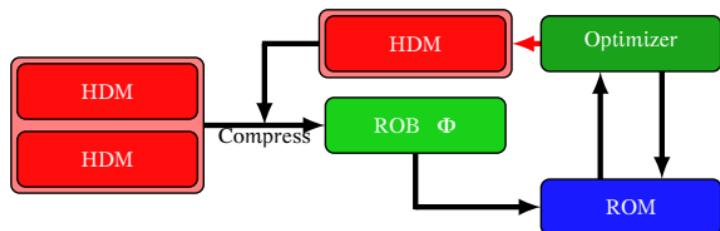
μ -space



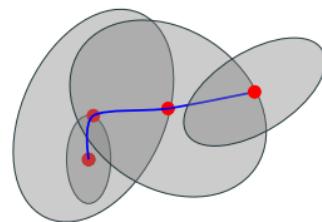
Breakdown of Computational Effort



Trust region framework for optimization with ROMs



Schematic



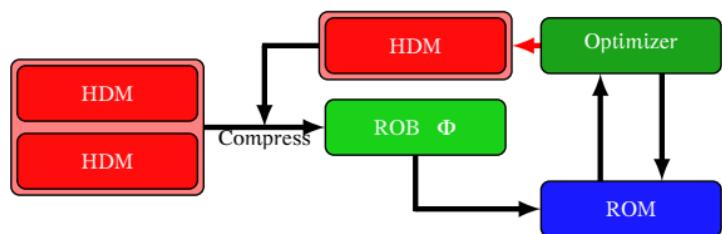
μ -space



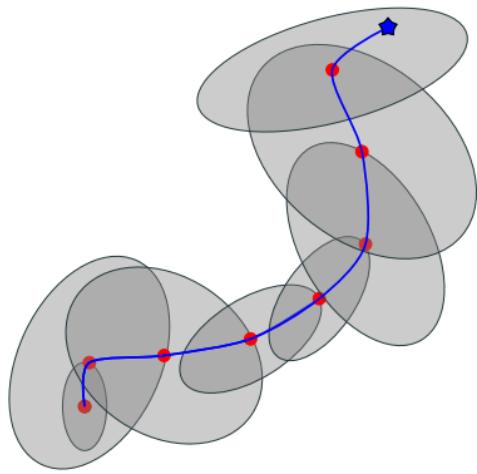
Breakdown of Computational Effort



Trust region framework for optimization with ROMs



Schematic



μ -space



Breakdown of Computational Effort



Trust region ingredients for global convergence

Approximation models

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

Error indicators

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

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

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

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

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



Trust region method: ROM approximation model

Approximation models based on reduced-order models

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

Error indicators from residual-based error bounds

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

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

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

Adaptivity to refine basis at trust region center

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

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

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



Trust region method: ROM approximation model

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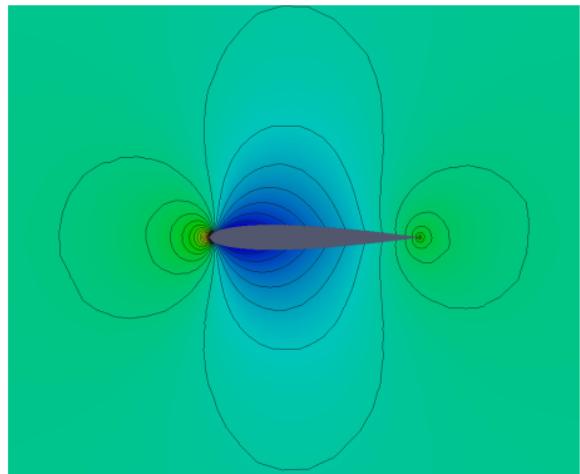
Interpolation property $\implies \vartheta_k(\mu_k) = \varphi_k(\mu_k) = 0$

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

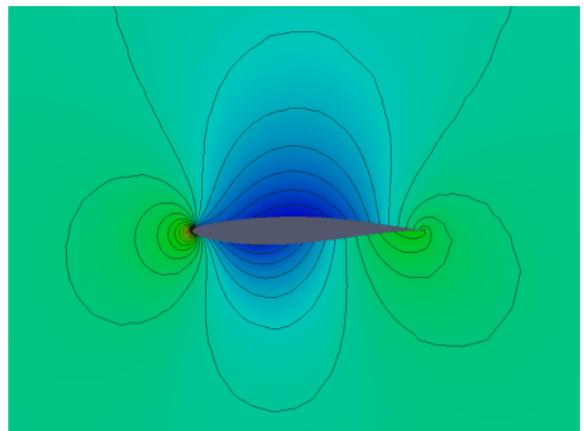


Compressible, inviscid airfoil design

Pressure discrepancy minimization (Euler equations)



NACA0012: Initial

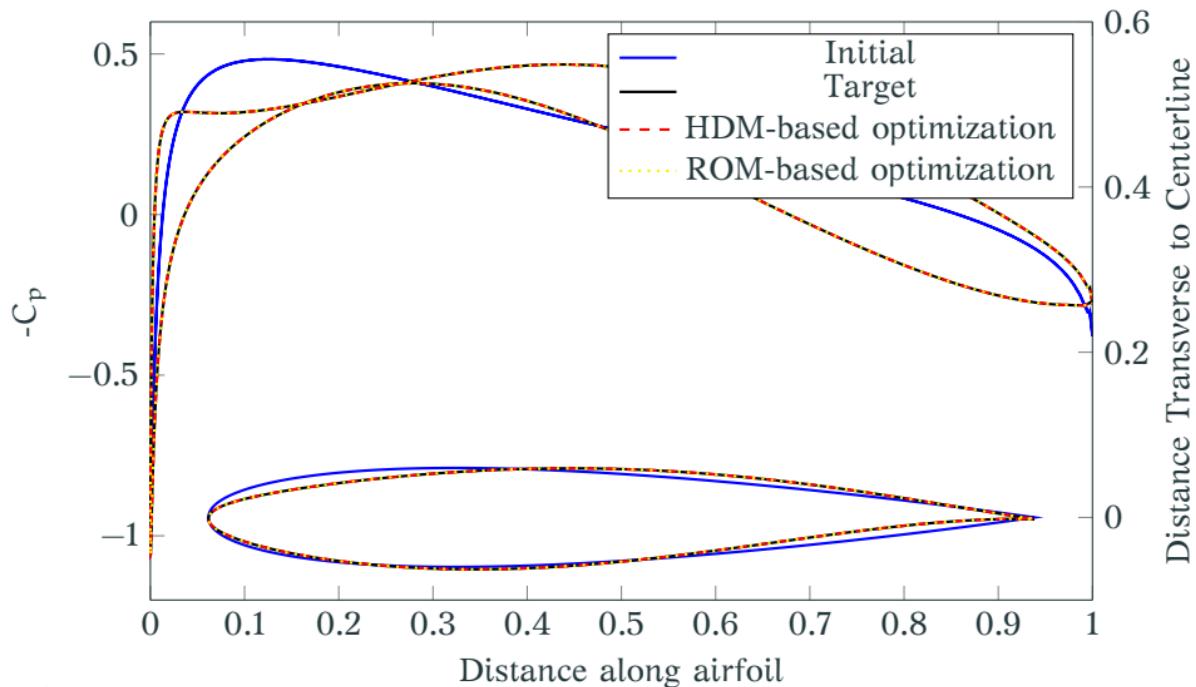


RAE2822: Target

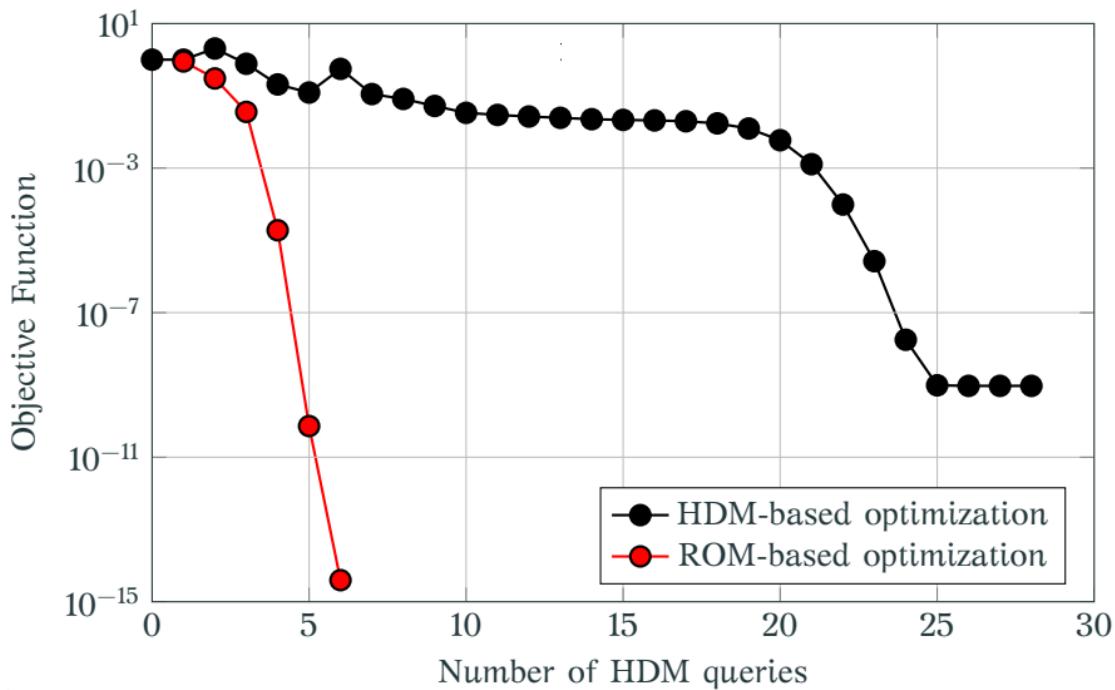
Pressure field for airfoil configurations at $M_{\infty} = 0.5$, $\alpha = 0.0^\circ$



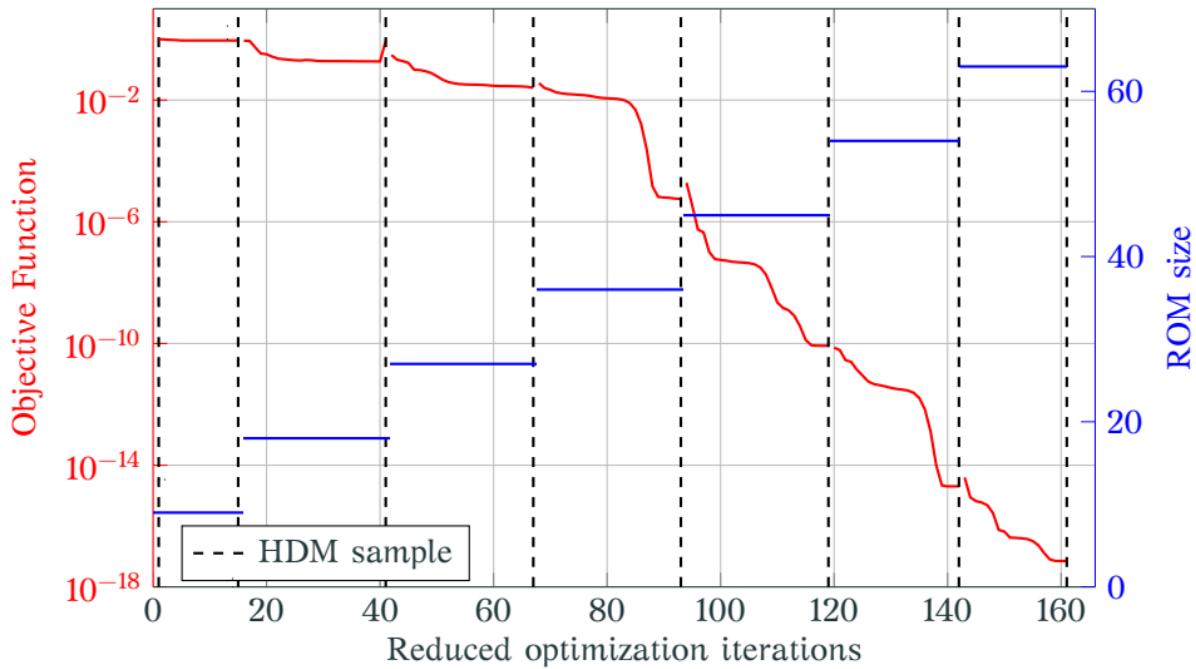
Proposed method: recovers target airfoil



Proposed method: $4\times$ fewer HDM queries



At the cost of ROM queries



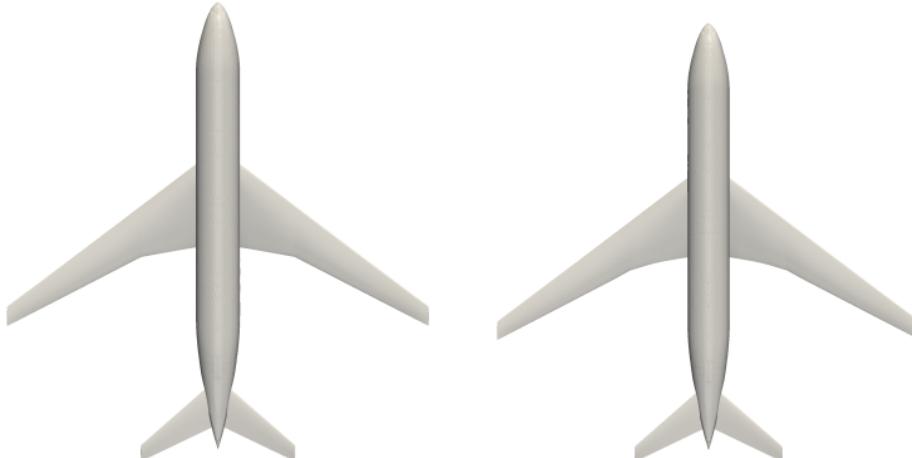
Shape optimization of aircraft in turbulent flow

$$\underset{\mu \in \mathbb{R}^4}{\text{minimize}} \quad -L_z(\mu)/L_x(\mu)$$

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

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

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



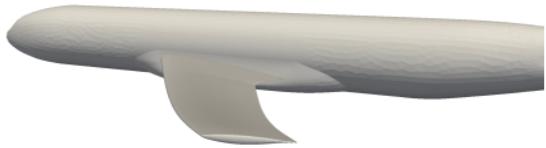
Shape optimization of aircraft in turbulent flow

minimize $\mu \in \mathbb{R}^4$ $- L_z(\mu) / L_x(\mu)$

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



Localized sweep



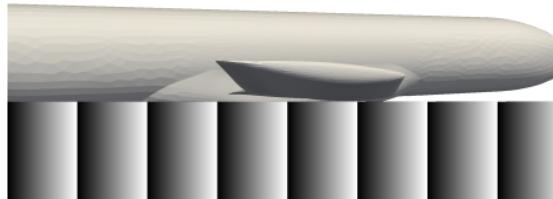
Shape optimization of aircraft in turbulent flow

$$\underset{\mu \in \mathbb{R}^4}{\text{minimize}} \quad -L_z(\mu)/L_x(\mu)$$

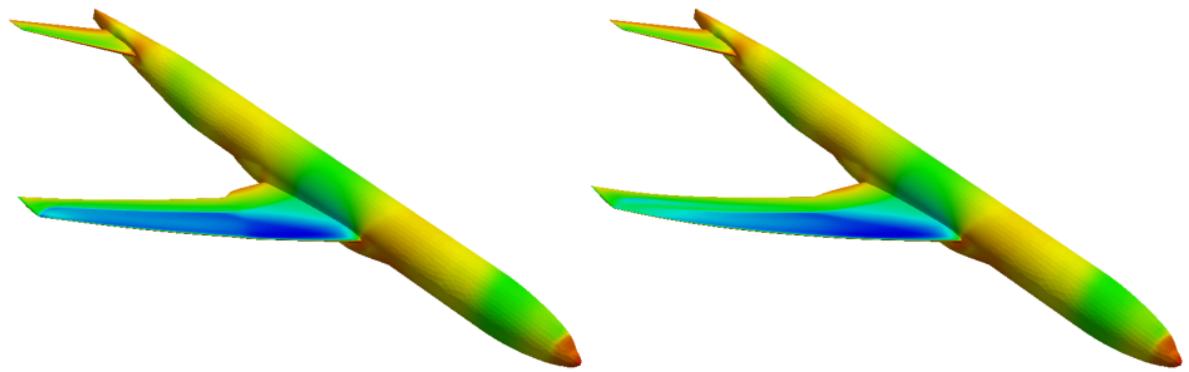
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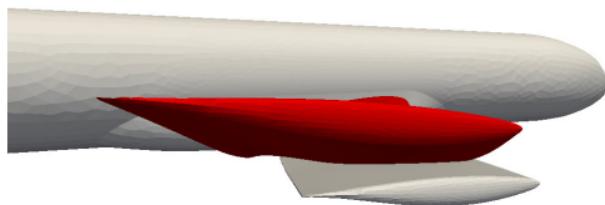
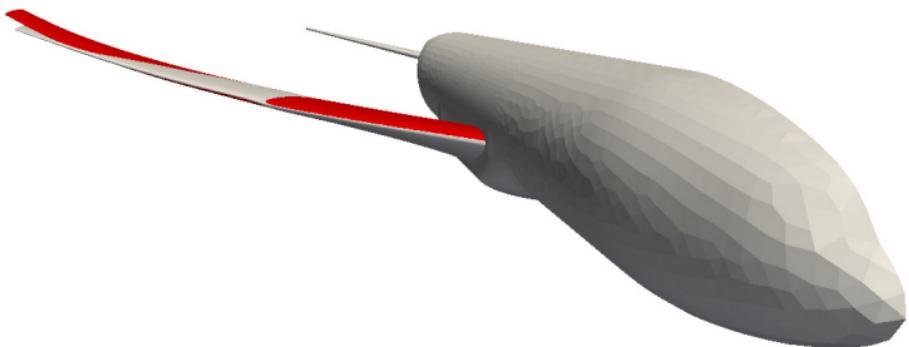
Optimized shape: reduction in 2.2 drag counts



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



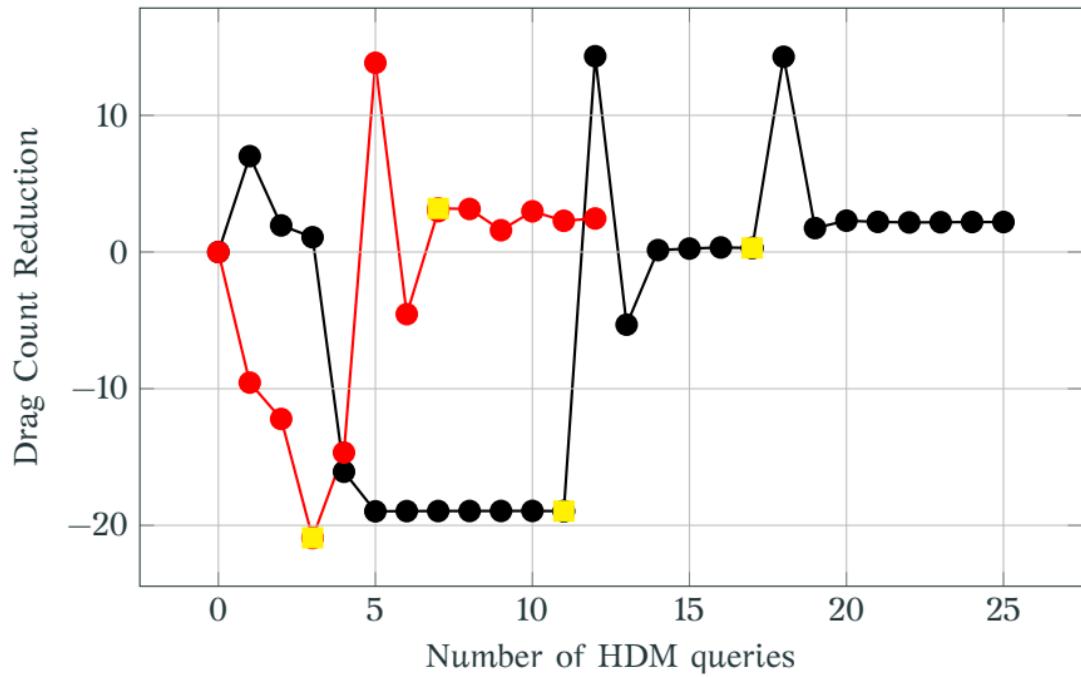
Optimized shape: reduction in 2.2 drag counts



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



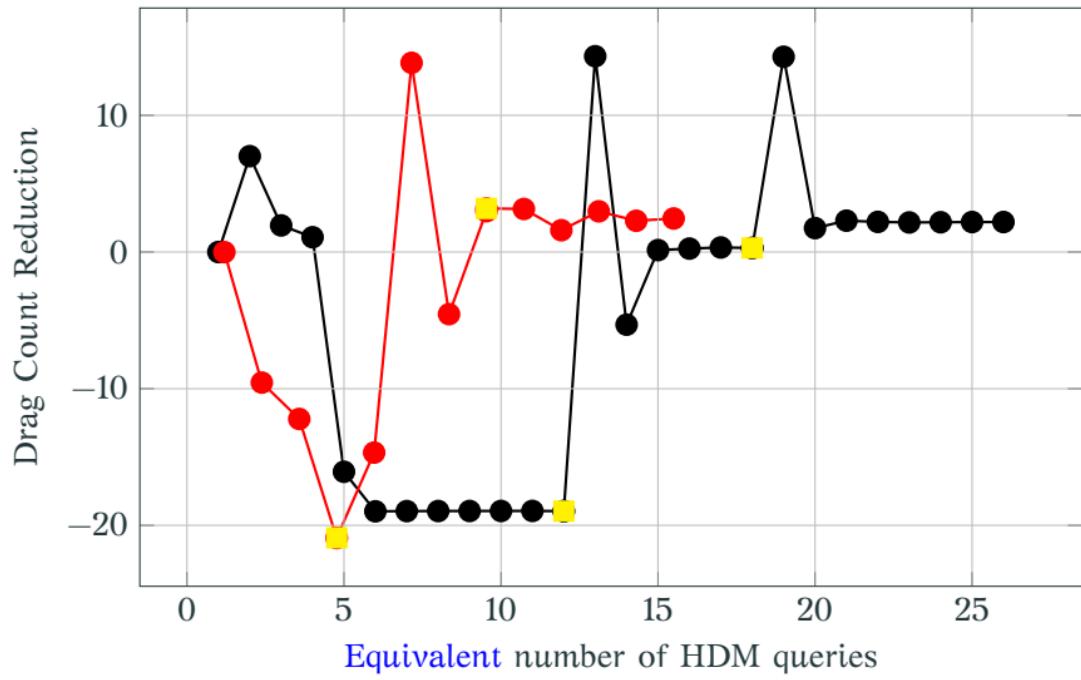
Proposed method: 2x reduction in number of HDM queries



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



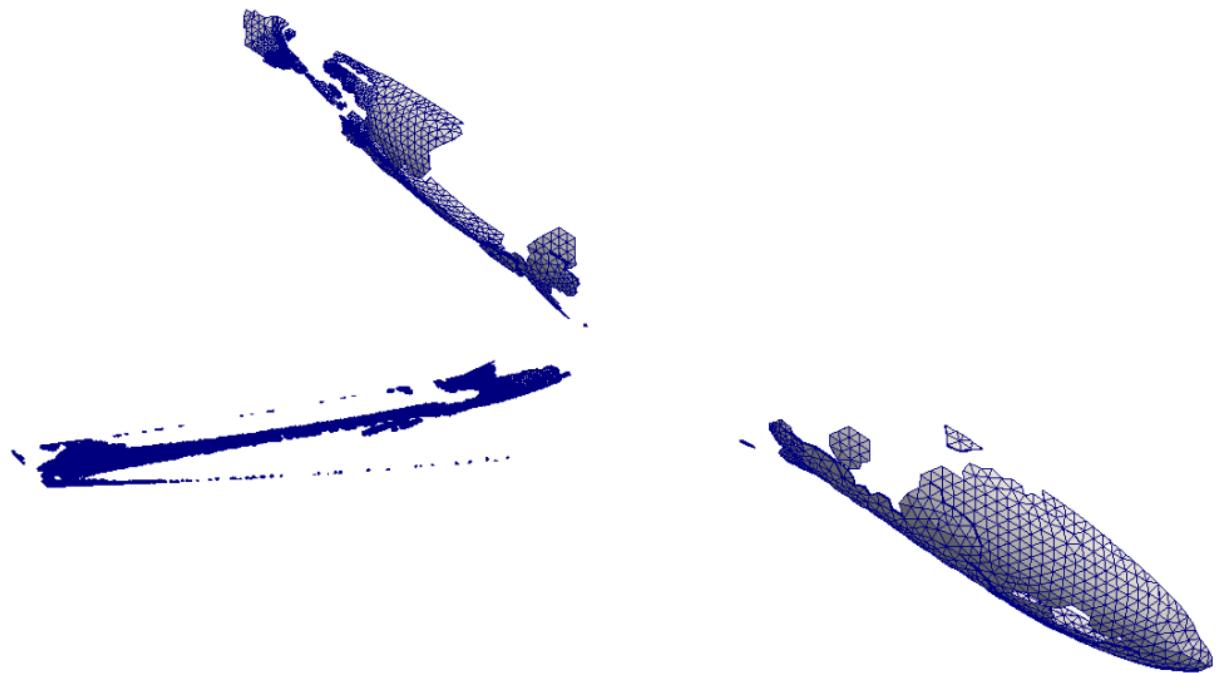
Proposed method: 1.6x reduction in overall cost



(—●—) 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

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

- $\mathbf{r} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \times \mathbb{R}^{n_\xi} \rightarrow \mathbb{R}^{n_u}$ discretized stochastic PDE
- $\mathcal{J} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \times \mathbb{R}^{n_\xi} \rightarrow \mathbb{R}$ 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
- $\mathbb{E}[\mathcal{F}] \equiv \int_{\Xi} \mathcal{F}(\boldsymbol{\xi}) \rho(\boldsymbol{\xi}) d\boldsymbol{\xi}$



First source of inexactness: anisotropic sparse grids

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

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



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

[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

$$\underset{\mathbf{u} \in \mathbb{R}^{n_u}, \mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad \mathbb{E}[\mathcal{J}(\mathbf{u}, \mu, \cdot)]$$

$$\text{subject to} \quad \mathbf{r}(\mathbf{u}, \mu, \xi) = 0 \quad \forall \xi \in \Xi$$



$$\underset{\mathbf{u} \in \mathbb{R}^{n_u}, \mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad \mathbb{E}_{\mathcal{I}}[\mathcal{J}(\mathbf{u}, \mu, \cdot)]$$

$$\text{subject to} \quad \mathbf{r}(\mathbf{u}, \mu, \xi) = 0 \quad \forall \xi \in \Xi_{\mathcal{I}}$$



$$\underset{\mathbf{u}_r \in \mathbb{R}^{k_u}, \mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad \mathbb{E}_{\mathcal{I}}[\mathcal{J}(\Phi \mathbf{u}_r, \mu, \cdot)]$$

$$\text{subject to} \quad \Psi^T \mathbf{r}(\Phi \mathbf{u}_r, \mu, \xi) = 0 \quad \forall \xi \in \Xi_{\mathcal{I}}$$



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

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

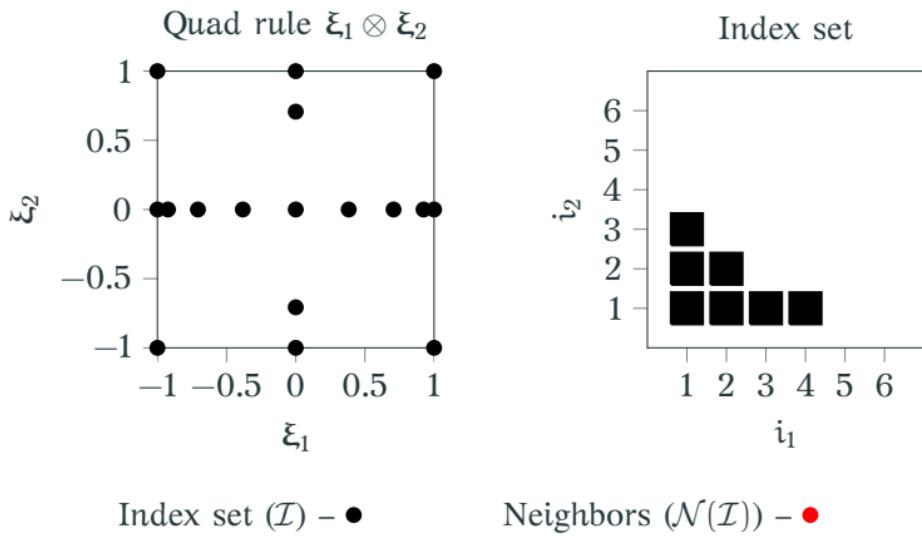
Manage inexactness with trust region method

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

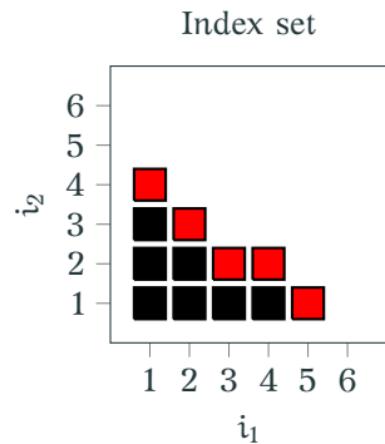
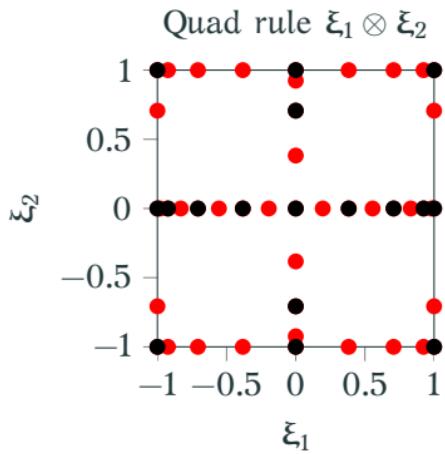
$$\underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad F(\mu) \quad \longrightarrow \quad \begin{array}{l} \underset{\mu \in \mathbb{R}^{n_\mu}}{\text{minimize}} \quad m_k(\mu) \\ \text{subject to} \quad \|\mu - \mu_k\| \leq \Delta_k \end{array}$$



Source of inexactness: anisotropic sparse grids



Source of inexactness: anisotropic sparse grids



Trust region method: ROM/SG approximation model

Approximation models built on two sources of inexactness

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

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

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

$$\mathcal{E}_1(\mu; \mathcal{I}, \Phi) = \mathbb{E}_{\mathcal{I} \cup \mathcal{N}(\mathcal{I})} [\|\mathbf{r}(\Phi u_r(\mu, \cdot), \mu, \cdot)\|]$$

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

Sparse grid truncation errors

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

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



Final requirement for convergence: Adaptivity

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

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

$$\varphi_k(\mu) = \alpha_1 \mathcal{E}_1(\mu; \mathcal{I}_k, \Phi_k) + \alpha_2 \mathcal{E}_2(\mu; \mathcal{I}_k, \Phi_k) + \alpha_3 \mathcal{E}_4(\mu; \mathcal{I}_k, \Phi_k)$$

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

$$\mathcal{E}_1(\mu_k; \mathcal{I}, \Phi) \leq \frac{\kappa_\varphi}{3\alpha_1} \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$$

$$\mathcal{E}_2(\mu_k; \mathcal{I}, \Phi) \leq \frac{\kappa_\varphi}{3\alpha_2} \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$$

$$\mathcal{E}_4(\mu_k; \mathcal{I}, \Phi) \leq \frac{\kappa_\varphi}{3\alpha_3} \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$$



Adaptivity: Dimension-adaptive greedy method

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

Refine index set: Dimension-adaptive sparse grids

$$\mathcal{I}_k \leftarrow \mathcal{I}_k \cup \{j^*\} \quad \text{where} \quad j^* = \arg \max_{j \in \mathcal{N}(\mathcal{I}_k)} \mathbb{E}_j [\|\nabla \mathcal{J}(\Phi u_r(\mu, \cdot), \mu, \cdot)\|]$$



Adaptivity: Dimension-adaptive greedy method

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

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Refine reduced-order basis: Greedy sampling

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

$$\Phi_k \leftarrow \begin{bmatrix} \Phi_k & u(\mu_k, \xi^*) & \lambda(\mu_k, \xi^*) \end{bmatrix}$$

$$\xi^* = \arg \max_{\xi \in \Xi_{j^*}} \rho(\xi) \|r(\Phi_k u_r(\mu_k, \xi), \mu_k, \xi)\|$$

end while



Adaptivity: Dimension-adaptive greedy method

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

Refine index set: Dimension-adaptive sparse grids

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$$\xi^* = \arg \max_{\xi \in \Xi_{j^*}} \rho(\xi) \|r(\Phi_k u_r(\mu_k, \xi), \mu_k, \xi)\|$$

end while

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

$$\Phi_k \leftarrow \begin{bmatrix} \Phi_k & u(\mu_k, \xi^*) & \lambda(\mu_k, \xi^*) \end{bmatrix}$$

$$\xi^* = \arg \max_{\xi \in \Xi_{j^*}} \rho(\xi) \|r^\lambda(\Phi_k u_r(\mu_k, \xi), \Psi_k \lambda_r(\mu_k, \xi), \mu_k, \xi)\|$$

end while



Optimal control of steady Burgers' equation

- Optimization problem:

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

where $u(\boldsymbol{\mu}, \xi, x)$ solves

$$\begin{aligned} -v(\xi) \partial_{xx} u(\boldsymbol{\mu}, \xi, x) + u(\boldsymbol{\mu}, \xi, x) \partial_x u(\boldsymbol{\mu}, \xi, x) &= z(\boldsymbol{\mu}, x) \quad x \in (0, 1), \quad \xi \in \Xi \\ u(\boldsymbol{\mu}, \xi, 0) &= d_0(\xi) \quad u(\boldsymbol{\mu}, \xi, 1) = d_1(\xi) \end{aligned}$$

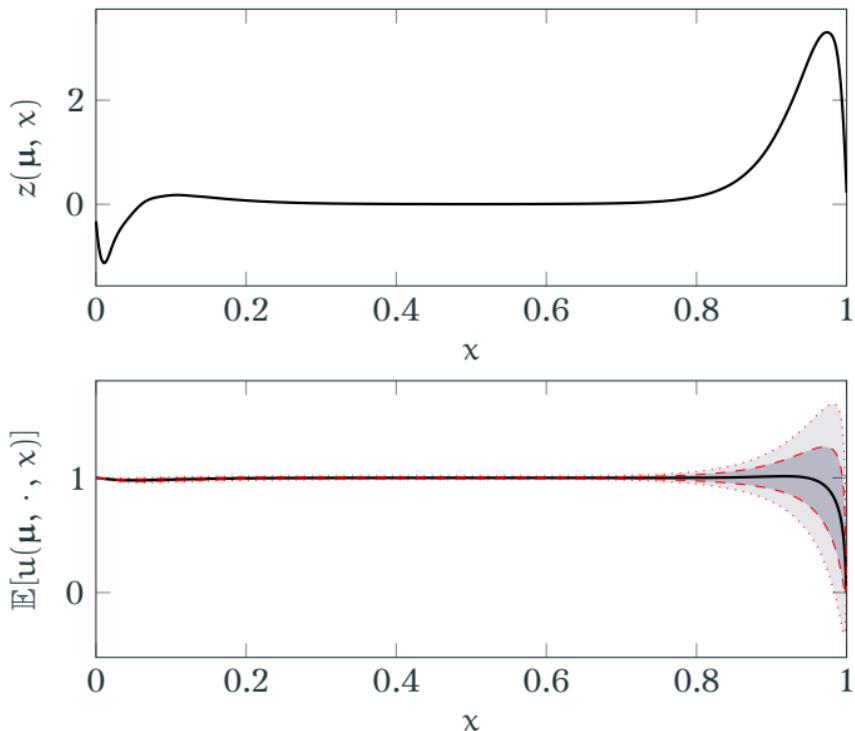
- Target state: $u(x) \equiv 1$
- Stochastic Space: $\Xi = [-1, 1]^3$, $\rho(\xi) d\xi = 2^{-3} d\xi$

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

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

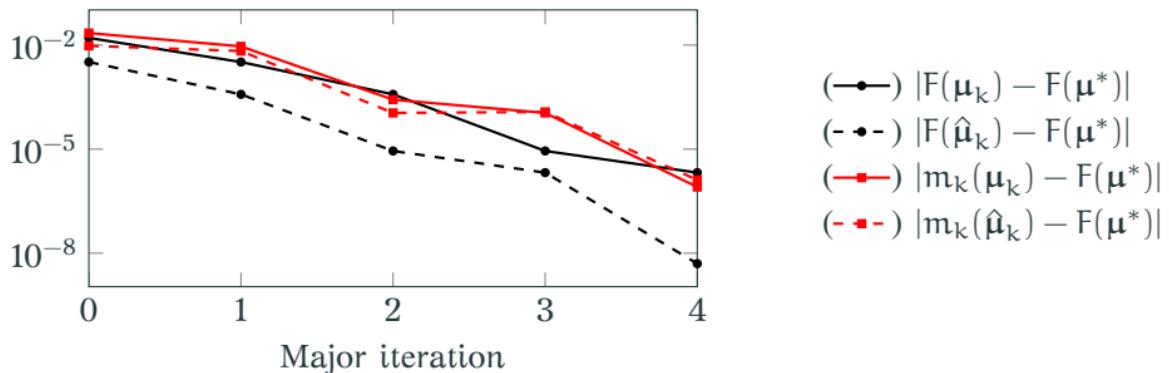


Optimal control and statistics



Optimal control and corresponding mean state (—) \pm one (---) and two (....) standard deviations

Global convergence without pointwise agreement



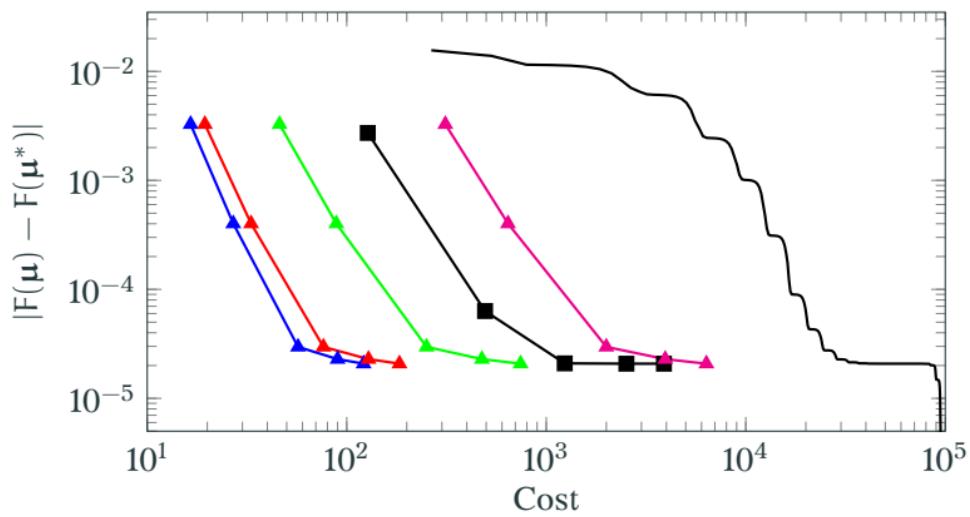
$F(\mu_k)$	$m_k(\mu_k)$	$F(\hat{\mu}_k)$	$m_k(\hat{\mu}_k)$	$\ \nabla F(\mu_k)\ $	ρ_k	Success?
6.6506e-02	7.2694e-02	5.3655e-02	5.9922e-02	2.2959e-02	1.0257e+00	1.0000e+00
5.3655e-02	5.9593e-02	5.0783e-02	5.7152e-02	2.3424e-03	9.7512e-01	1.0000e+00
5.0783e-02	5.0670e-02	5.0412e-02	5.0292e-02	1.9724e-03	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 \times faster than HDM

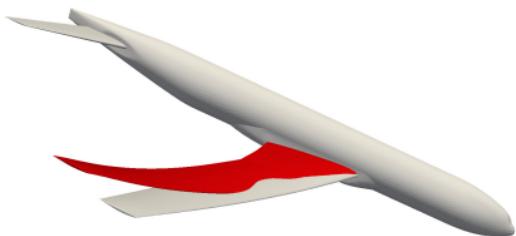
$$\text{Cost} = n\text{HdmPrim} + 0.5 \times n\text{HdmAdj} + \tau^{-1} \times (n\text{RomPrim} + 0.5 \times n\text{RomAdj})$$



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

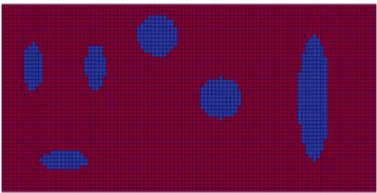
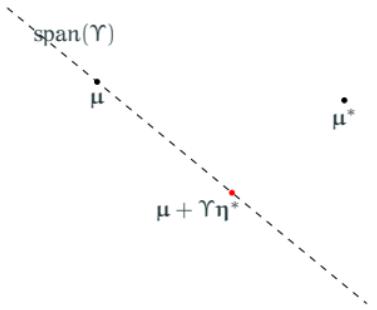
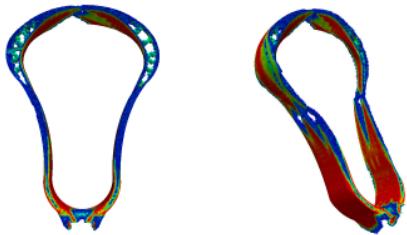
Leveraging inexactness to accelerate PDE-constrained optimization

- 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
 - $1.6\times$ speedup on (deterministic) shape design of aircraft
 - $100\times$ speedup on (stochastic) optimal control of 1D flow

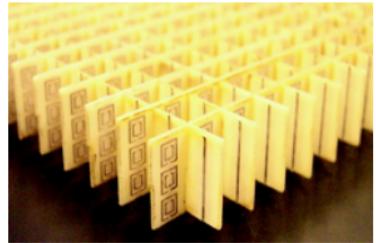
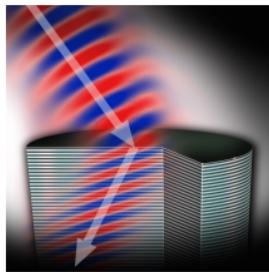


Extension to problems with many parameters

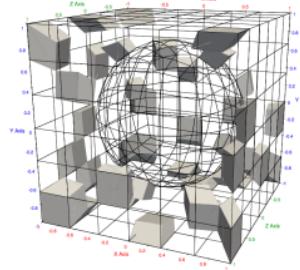
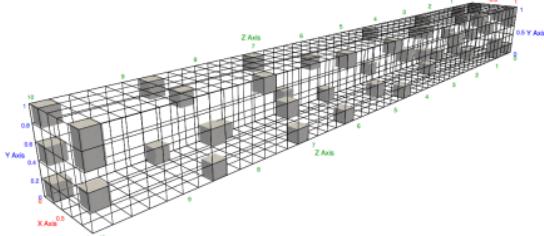
- Topology optimization³ and inverse problems
- **Nested reduction** of state and parameter
- Multifidelity trust region method to globalize **state** reduction
- Linesearch/subspace method to globalize **parameter** reduction



Extension to multiscale problems

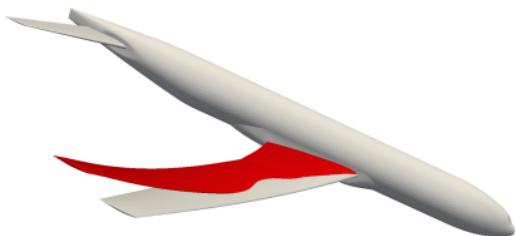


- **Existing multiscale methods** are extremely expensive
 - Single simulation: 203 hours (\approx 8.5 days), 41760 cores [Knap et. al., 2016]
 - Not amenable to optimization (many-query)
- **Hyperreduced models** at each scale [Zahr et al., 2016a] – embedded in trust region optimization framework to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



Leveraging inexactness to accelerate PDE-constrained optimization

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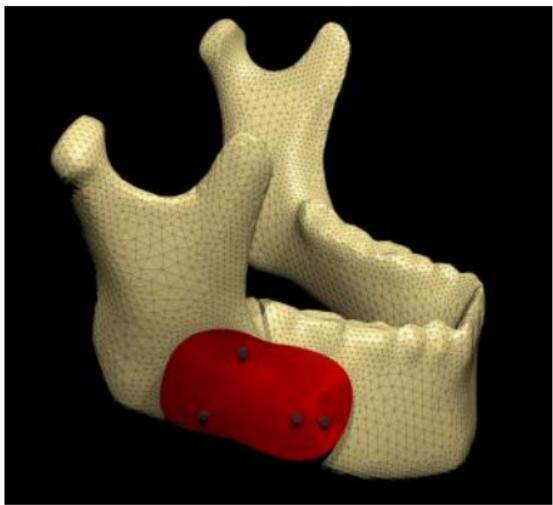
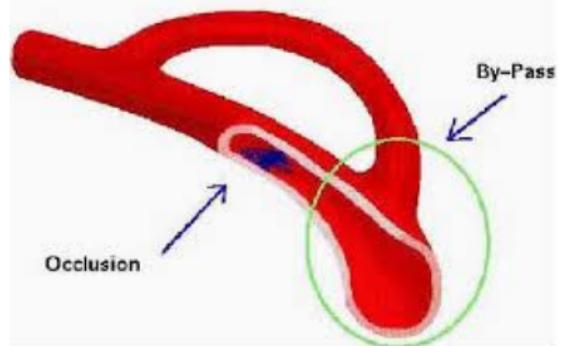
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Computers & Fluids.



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 theory⁴

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: $\Delta_k \rightarrow 0$

- 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: $\rho_k \rightarrow 1$

- 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 $\implies \liminf \|\nabla m_k(\mu_k)\| = 0$
- $\|\nabla F(\mu_k) - \nabla m_k(\mu_k)\| \leq \xi \min\{\|\nabla m_k(\mu)\|, \Delta_k\}$



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 ($\boldsymbol{\Theta} = \mathbf{I}$)

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

- + 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

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

- + **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 sensitivity⁵

These quantities agree if $\Phi^\partial = \Phi$ and either Ψ is constant or the primal ROM is exact
Lahr et al., 2016b]

Hyperreduction to reduce complexity of nonlinear terms

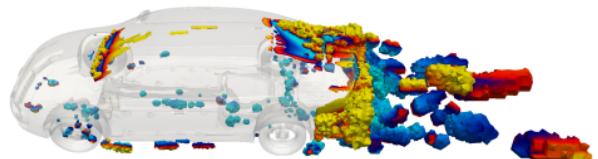
Despite reduced dimensionality, $\mathcal{O}(n_u)$ operations are required to evaluate

$$\Psi^T r(\Phi u_r, \mu) \quad \Psi^T \frac{\partial r}{\partial u}(\Phi u_r, \mu) \Phi$$

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

$$\underset{u_r \in \mathbb{R}^{k_u}}{\text{minimize}} \quad \|r(\Phi u_r, \mu)\|_{\Theta} \implies \underset{u_r \in \mathbb{R}^{k_u}}{\text{minimize}} \quad \left\| P^T r(\Phi u_r, \mu) \right\|_{\Theta}$$

and **hyperreduced** model⁶ is independent of n_u



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



lacked 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

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

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*

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



Source of inexactness: Partially Converged Solution (PCS)

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

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

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

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



Trust region method: ROM/PCS approximation model

Approximation models based on ROMs and partially converged solutions

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

Error indicators from residual-based error bounds

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

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

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

Adaptivity to refine basis at trust region center

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

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

and $\alpha_k, \beta_k, \tau_k$ selected such that

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

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



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Error indicators from residual-based error bounds

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

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

Adaptivity to refine basis at trust region center

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

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

and $\alpha_k, \beta_k, \tau_k$ selected such that

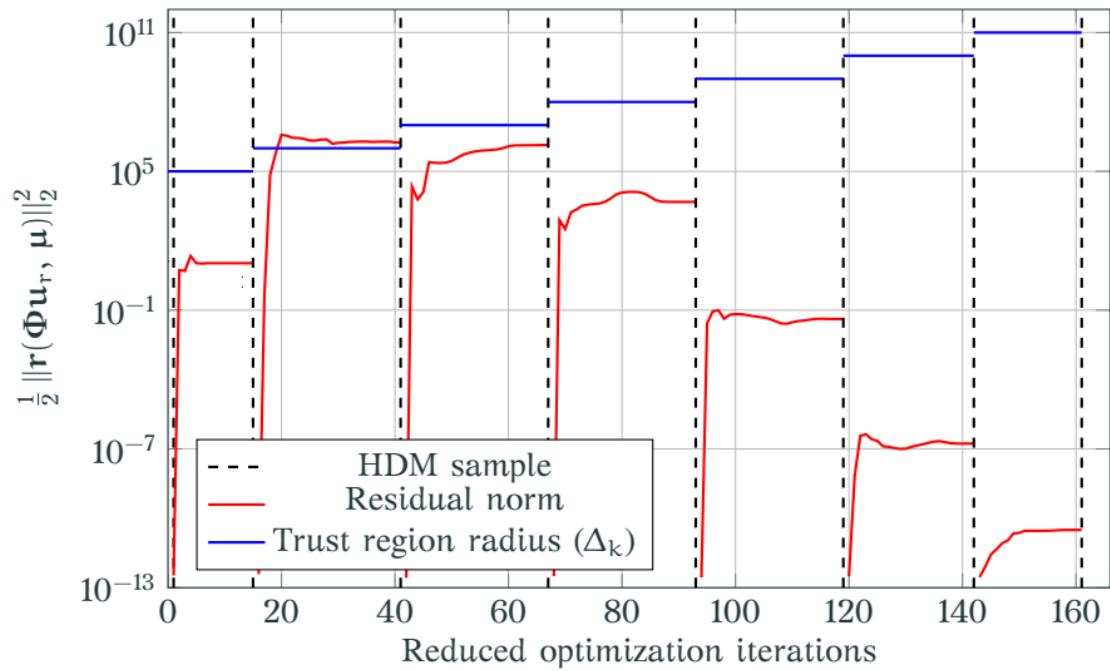
$$\vartheta_k(\mu_k) \leq \kappa_{\vartheta} \Delta_k \quad \varphi_k(\mu_k) \leq \kappa_{\varphi} \min\{\|\nabla m_k(\mu_k)\|, \Delta_k\}$$

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

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



Error-aware trust region behavior



Source of inexactness: anisotropic sparse grids

1D Quadrature Rules: Define the difference operator

$$\Delta_k^j \equiv E_k^j - E_k^{j-1}$$

where $E_k^0 \equiv 0$ and 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

$$E_{\mathcal{I}} \equiv \sum_{i \in \mathcal{I}} \Delta_1^{i_1} \otimes \cdots \otimes \Delta_{n_\xi}^{i_{n_\xi}}$$

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

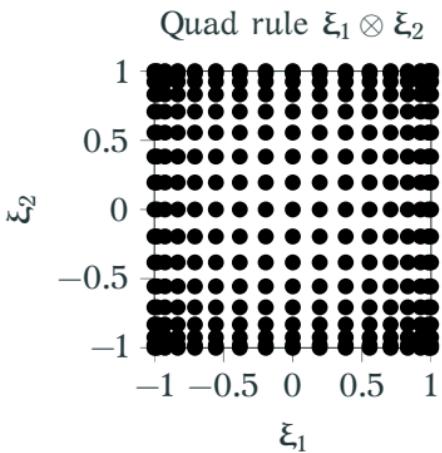
$$\mathcal{N}(\mathcal{I}) = \{i \in \mathcal{I}^c \mid i - e_j \in \mathcal{I}, j = 1, \dots, n_\xi\}$$

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

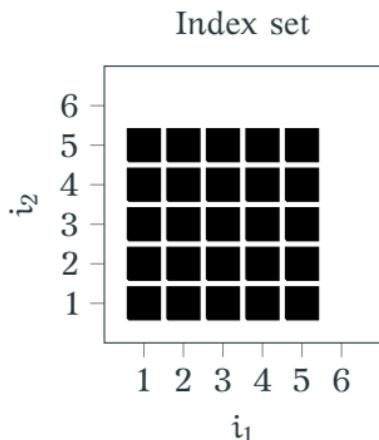
$$E - E_{\mathcal{I}} = \sum_{i \in \mathcal{I}^c} \Delta_1^{i_1} \otimes \cdots \otimes \Delta_{n_\xi}^{i_{n_\xi}} \approx \sum_{i \in \mathcal{N}(\mathcal{I})} \Delta_1^{i_1} \otimes \cdots \otimes \Delta_{n_\xi}^{i_{n_\xi}} = E_{\mathcal{N}(\mathcal{I})}$$



Tensor product quadrature



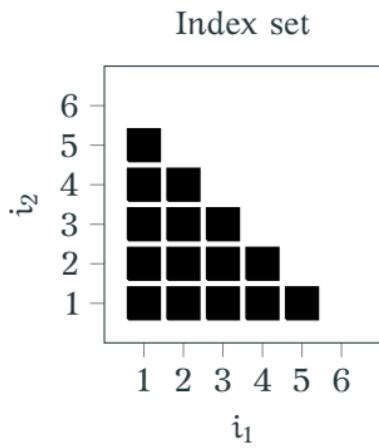
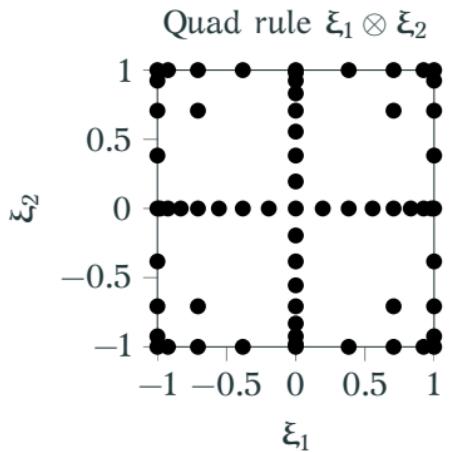
Index set (\mathcal{I}) – ●



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



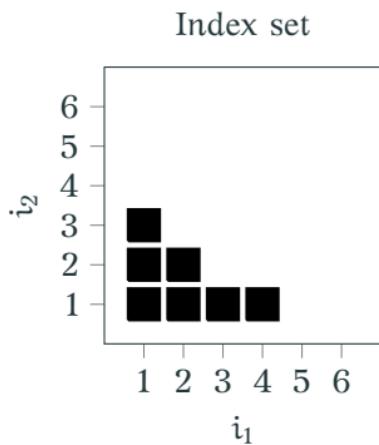
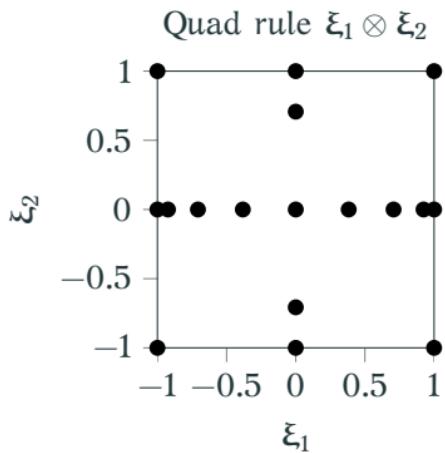
Isotropic sparse grid quadrature



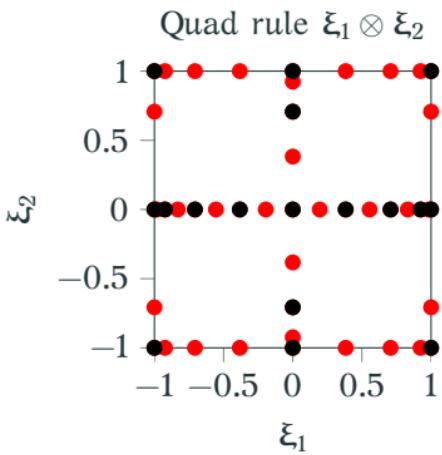
Neighbors ($\mathcal{N}(\mathcal{I})$) – ●



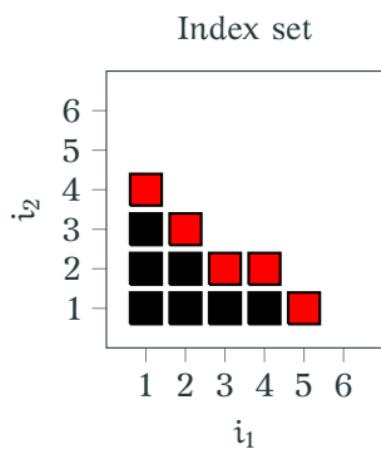
Anisotropic sparse grid quadrature



Anisotropic sparse grid quadrature: neighbors



Index set (\mathcal{I}) – ●



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



Derivation of gradient error indicator

For brevity, let

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

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

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

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

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

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

Separate total error into contributions from **ROM inexactness** and **SG truncation**

$$\|\mathbb{E}[\nabla \mathcal{J}] - \mathbb{E}_{\mathcal{I}}[\nabla \mathcal{J}_r]\| \leq \textcolor{red}{\|\mathbb{E}[\nabla \mathcal{J} - \nabla \mathcal{J}_r]\|} + \textcolor{blue}{\|\mathbb{E}[\nabla \mathcal{J}_r] - \mathbb{E}_{\mathcal{I}}[\nabla \mathcal{J}_r]\|}$$



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Separate total error into contributions from **ROM inexactness** and **SG truncation**

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



Derivation of gradient error indicator

For brevity, let

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

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

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

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

Separate total error into contributions from ROM inexactness and SG truncation

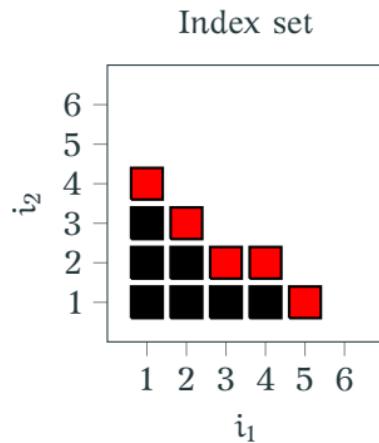
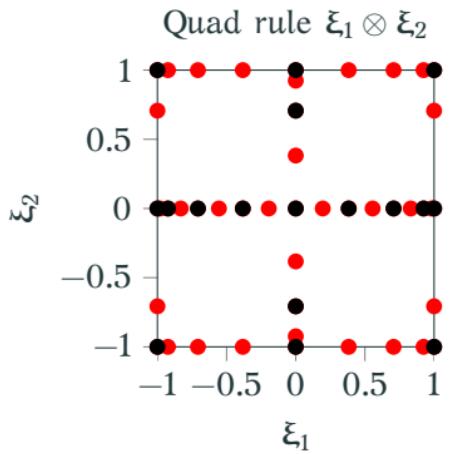
$$\|\mathbb{E}[\nabla \mathcal{J}] - \mathbb{E}_{\mathcal{I}}[\nabla \mathcal{J}_r]\| \leq \mathbb{E} [\|\nabla \mathcal{J} - \nabla \mathcal{J}_r\|] + \|\mathbb{E}[\nabla \mathcal{J}_r] - \mathbb{E}_{\mathcal{I}}[\nabla \mathcal{J}_r]\|$$

$$\leq \zeta' \mathbb{E} [\alpha_1 \|\mathbf{r}\| + \alpha_2 \|\mathbf{r}^\lambda\|] + \mathbb{E}_{\mathcal{I}^c} [\|\nabla \mathcal{J}_r\|]$$

$$\lesssim \zeta (\mathbb{E}_{\mathcal{I} \cup \mathcal{N}(\mathcal{I})} [\alpha_1 \|\mathbf{r}\| + \alpha_2 \|\mathbf{r}^\lambda\|] + \alpha_3 \mathbb{E}_{\mathcal{N}(\mathcal{I})} [\|\nabla \mathcal{J}_r\|])$$



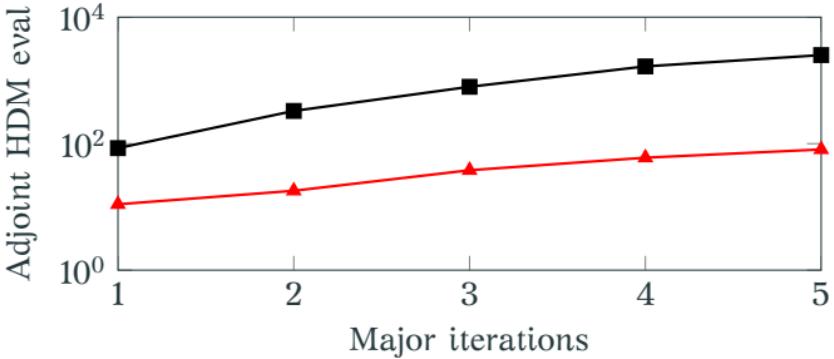
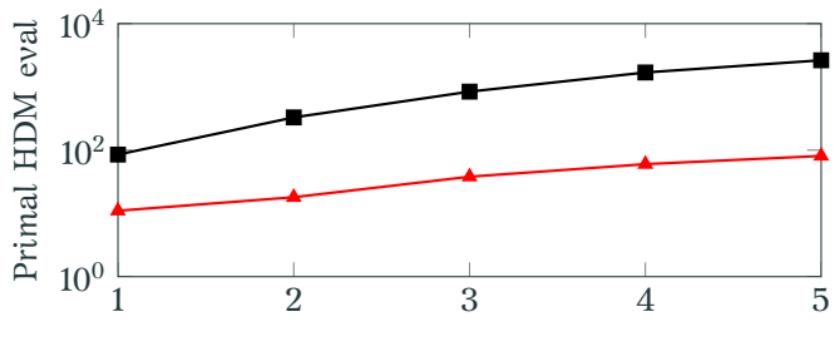
Adaptivity: Dimension-adaptive greedy method



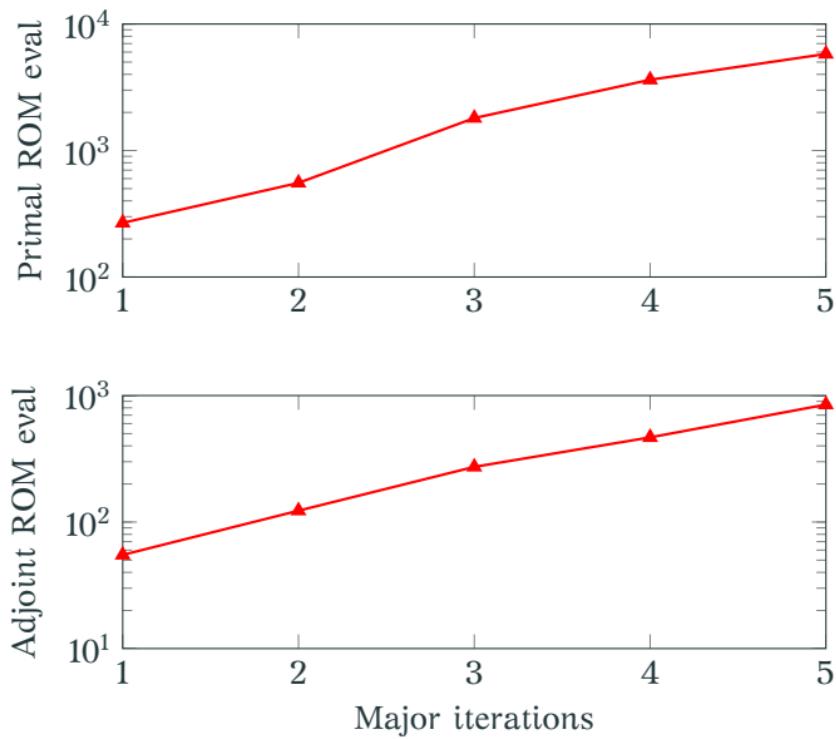
Significant reduction in number of queries to HDM in comparison to state-of-the-art [Kouri et al., 2014]

Adaptive SG (■)

Adaptive SG/ROM (▲)



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



Extension to time-dependent problems

- **Applications:** inverse problems, optimal flapping flight and swimming⁷ 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)



insight into bio-locomotion, design of micro-aerial vehicles

