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

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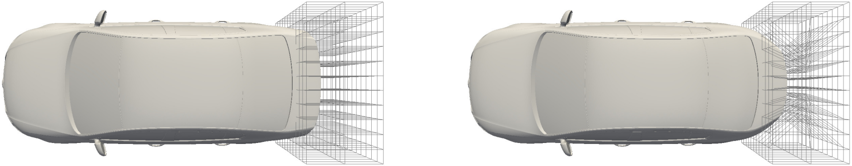
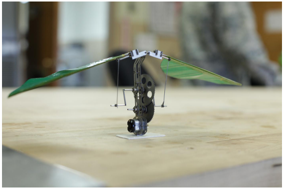
PDE optimization is **ubiquitous** in science and engineering

Design: Find system that optimizes performance metric, satisfies constraints



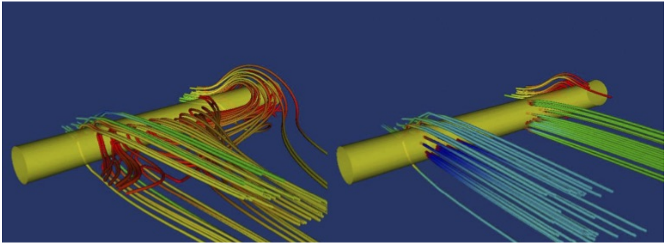
Aerodynamic shape design of automobile



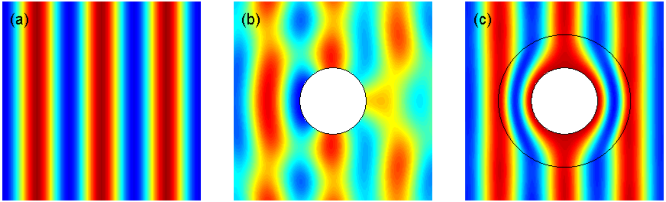
Optimal flapping motion of micro aerial vehicle

PDE optimization is **ubiquitous** in science and engineering

Control: Drive system to a desired state

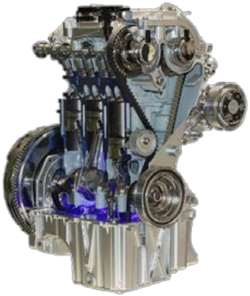


Boundary flow control

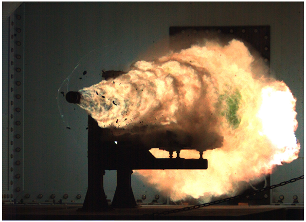


Metamaterial cloaking – electromagnetic invisibility

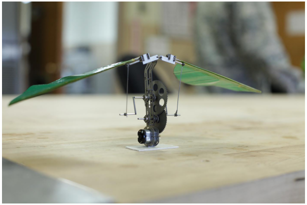
Current interest in ***computational physics*** *reaches far beyond analysis of a single configuration of a physical system into* ***design*** *(shape and topology) and* ***control*** *in an* ***uncertain*** *setting*



Engine System



EM Launcher



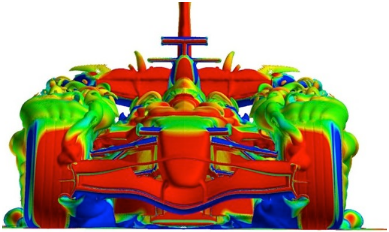
Micro-Aerial Vehicle

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

Deterministic PDE-constrained optimization formulation

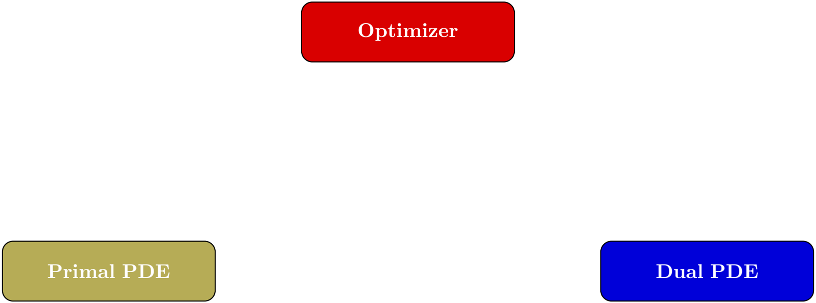
$$\begin{aligned} \underset{\boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathcal{J}(\boldsymbol{u},\, \boldsymbol{\mu}) \\ \text{subject to} \quad & \boldsymbol{r}(\boldsymbol{u};\, \boldsymbol{\mu}) = 0 \end{aligned}$$

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



Nested approach to PDE-constrained optimization

Virtually all expense emanates from primal/dual PDE solves



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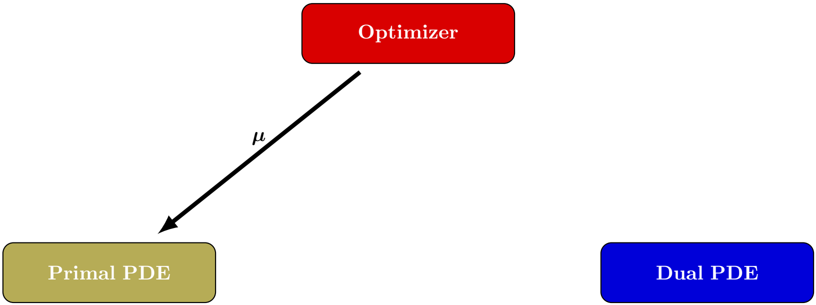

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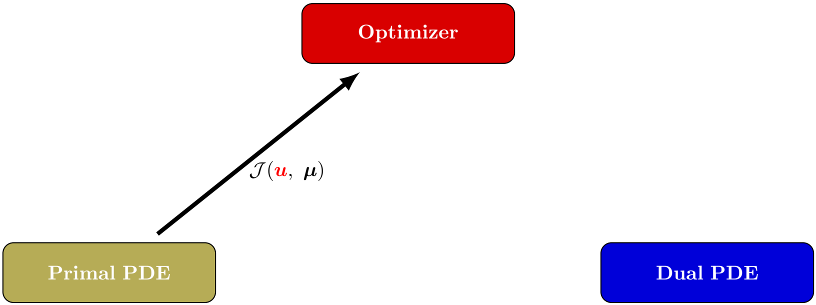

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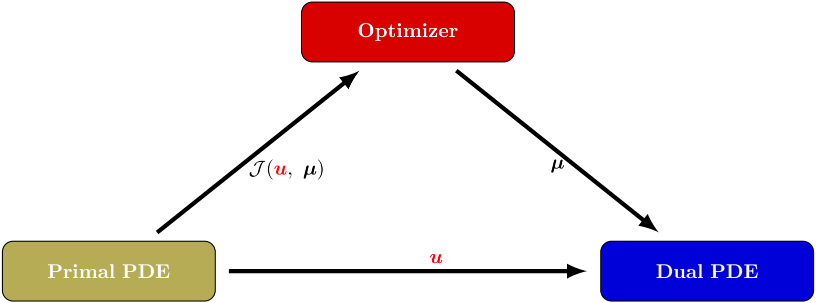

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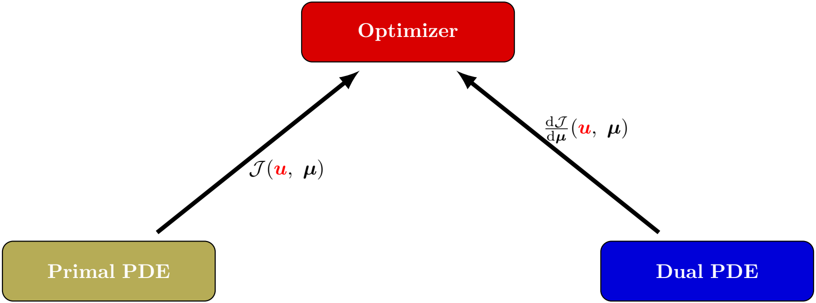


Applications in computational mechanics: static

Maximum lift-to-drag airfoil configuration

Stochastic PDE-constrained optimization formulation

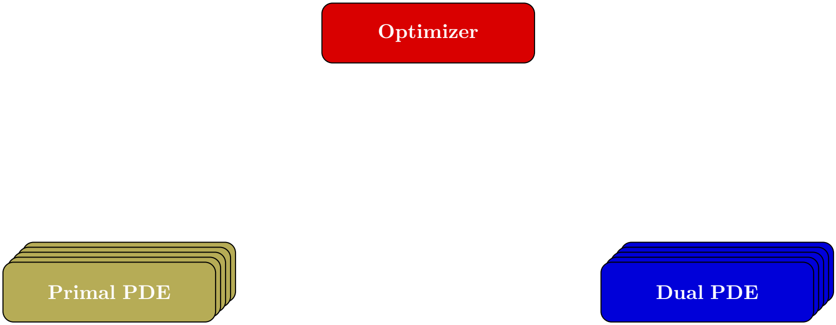
$$\begin{aligned} \underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathbb{E}[\mathcal{J}(\boldsymbol{u}, \boldsymbol{\mu}, \cdot)] \\ \text{subject to} \quad & \boldsymbol{r}(\boldsymbol{u}; \boldsymbol{\mu}, \boldsymbol{\xi}) = 0 \quad \forall \boldsymbol{\xi}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

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

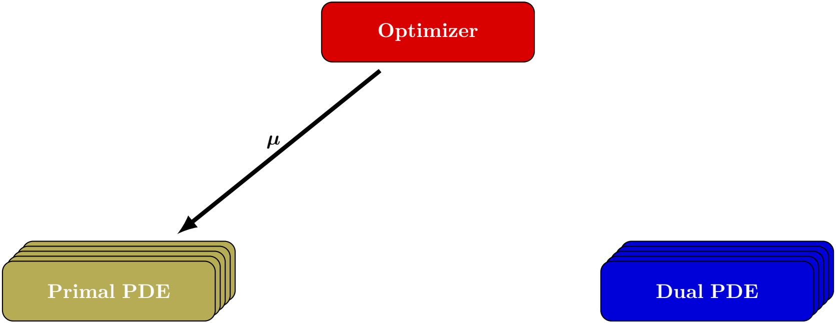
Each function evaluation requires integration over stochastic space – ***expensive***

Nested approach to stochastic PDE-constrained optimization

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



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



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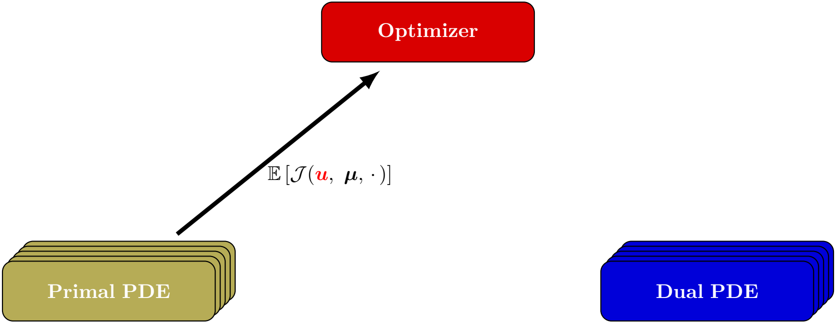

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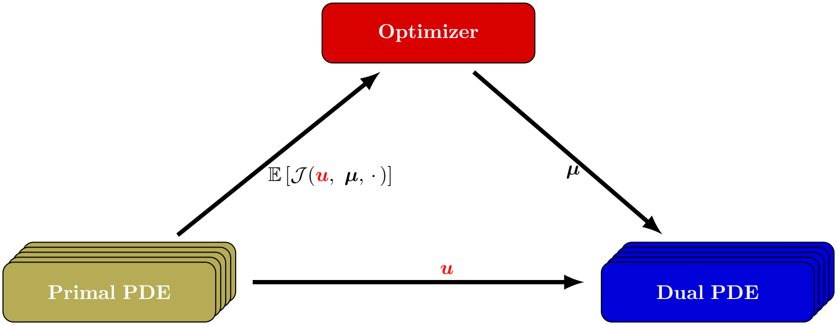
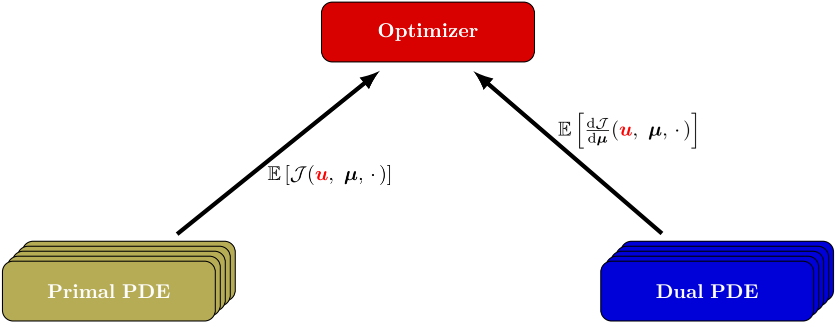


Ensemble** of primal/dual PDE solves increases cost by **orders of magnitude



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

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

[1] 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*

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

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

- First-order consistency [Alexandrov et al., 1998]

$$m_k(\boldsymbol{\mu}_k) = F(\boldsymbol{\mu}_k) \qquad \nabla m_k(\boldsymbol{\mu}_k) = \nabla F(\boldsymbol{\mu}_k)$$

- The Carter condition [Carter, 1989, Carter, 1991]

$$||\nabla F(\boldsymbol{\mu}_k) - \nabla m_k(\boldsymbol{\mu}_k)|| \leq \eta \, ||\nabla m_k(\boldsymbol{\mu}_k)|| \qquad \eta \in (0,\, 1)$$

- Asymptotic gradient bound [Heinkenschloss and Vicente, 2002]

$$||\nabla F(\boldsymbol{\mu}_k) - \nabla m_k(\boldsymbol{\mu}_k)|| \leq \xi \min\{||\nabla m_k(\boldsymbol{\mu}_k)|| \,,\, \Delta_k\} \qquad \xi > 0$$

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

$$||\nabla F(\boldsymbol{\mu}) - \nabla m_k(\boldsymbol{\mu})|| \leq \xi \varphi_k(\boldsymbol{\mu}) \qquad \xi > 0$$
$$\varphi_k(\boldsymbol{\mu}_k) \leq \kappa_\varphi \min\{||\nabla m_k(\boldsymbol{\mu}_k)|| \,,\, \Delta_k\}$$

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

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

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

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

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

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

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

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

4: **Trust region update**:

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

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

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

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

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

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

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

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

4: **Trust region update**:

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

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

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

Asymptotic accuracy requirements on approximation model [Zahr, 2016]

$$\begin{aligned} |F(\boldsymbol{\mu}_k) - F(\boldsymbol{\mu}) + m_k(\boldsymbol{\mu}) - m_k(\boldsymbol{\mu}_k)| &\leq \zeta \vartheta_k(\boldsymbol{\mu}) & \zeta &> 0 \\ \vartheta_k(\boldsymbol{\mu}_k) &\leq \kappa_\vartheta \Delta_k & \kappa_\vartheta &\in (0,\, 1) \end{aligned}$$

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

$$\begin{aligned} |F(\boldsymbol{\mu}_k) - F(\boldsymbol{\mu}) + \psi_k(\boldsymbol{\mu}) - \psi_k(\boldsymbol{\mu}_k)| &\leq \sigma \theta_k(\boldsymbol{\mu}) \qquad \sigma > 0 \\ \theta_k(\hat{\boldsymbol{\mu}}_k)^\omega &\leq \eta \min\{m_k(\boldsymbol{\mu}_k) - m_k(\hat{\boldsymbol{\mu}}_k),\, r_k\} \end{aligned}$$

$$\omega,\, \eta \in (0,\, 1),\, r_k \to 0$$

Trust region ingredients for **global convergence**

Approximation models

$$m_k(\boldsymbol{\mu}),\ \psi_k(\boldsymbol{\mu})$$

Error indicators

$$\begin{aligned}
|F(\boldsymbol{\mu}_k) - F(\boldsymbol{\mu}) + m_k(\boldsymbol{\mu}) - m_k(\boldsymbol{\mu}_k)| &\leq \zeta \vartheta_k(\boldsymbol{\mu}) & \zeta > 0 \\
||\nabla F(\boldsymbol{\mu}) - \nabla m_k(\boldsymbol{\mu})|| &\leq \xi \varphi_k(\boldsymbol{\mu}) & \xi > 0 \\
|F(\boldsymbol{\mu}_k) - F(\boldsymbol{\mu}) + \psi_k(\boldsymbol{\mu}) - \psi_k(\boldsymbol{\mu}_k)| &\leq \sigma \theta_k(\boldsymbol{\mu}) & \sigma > 0
\end{aligned}$$

Adaptivity

$$\begin{aligned}
\vartheta_k(\boldsymbol{\mu}_k) &\leq \kappa_\vartheta \Delta_k \\
\varphi_k(\boldsymbol{\mu}_k) &\leq \kappa_\varphi \min\{||\nabla m_k(\boldsymbol{\mu}_k)||\,,\ \Delta_k\} \\
\theta_k(\hat{\boldsymbol{\mu}}_k)^\omega &\leq \eta \min\{m_k(\boldsymbol{\mu}_k) - m_k(\hat{\boldsymbol{\mu}}_k),\ r_k\}
\end{aligned}$$

Global convergence

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

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Source of inexactness: **projection-based model reduction**

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

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

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

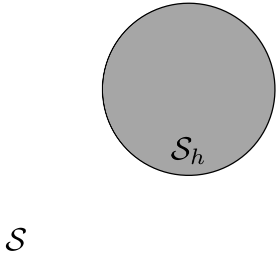
- Substitute into $\boldsymbol{r}(\boldsymbol{u},\, \boldsymbol{\mu}) = 0$ and project onto columnspace of a test basis $\boldsymbol{\Psi} \in \mathbb{R}^{n_{\boldsymbol{u}} \times k_{\boldsymbol{u}}}$ to obtain a square system

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

Connection to finite element method: hierarchical subspaces

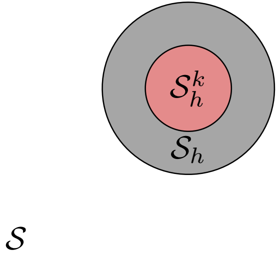
$$\mathcal{S}$$

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



- $\mathcal{S}$ - infinite-dimensional trial space
- $\mathcal{S}_h$ - (large) finite-dimensional trial space

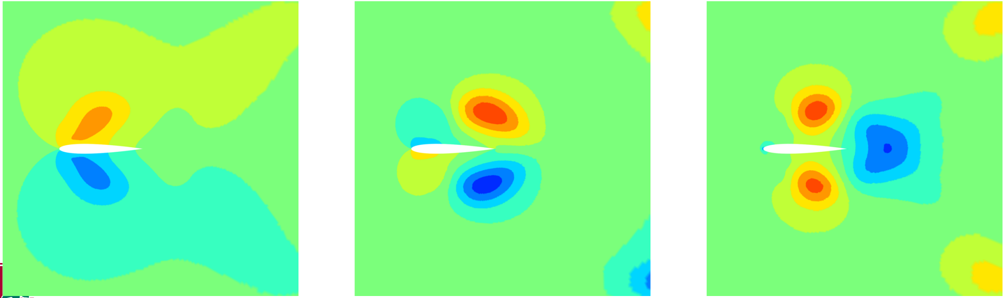
Connection to finite element method: hierarchical subspaces



- $\mathcal{S}$ - infinite-dimensional trial space
- $\mathcal{S}_h$ - (large) finite-dimensional trial space
- $\mathcal{S}_h^k$ - (small) finite-dimensional trial space
- $\mathcal{S}_h^k \subset \mathcal{S}_h \subset \mathcal{S}$

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 $\boldsymbol{\Psi}^T \boldsymbol{r}(\boldsymbol{\Phi}\boldsymbol{u}_r,\ \boldsymbol{\mu}) = 0$ is equivalent to the optimality condition of

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

which requires

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

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

Implications of the minimum-residual property

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

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

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

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

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

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

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

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

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

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

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

Minimum-residual sensitivity analysis

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

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

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

Hyperreduction to reduce complexity of nonlinear terms

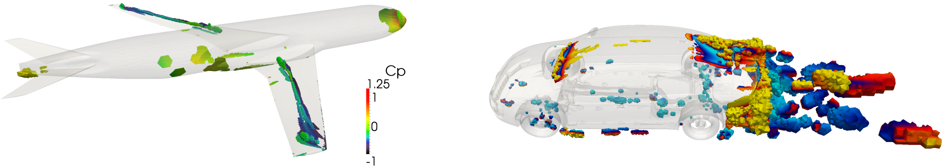
Despite **reduced dimensionality**, $\mathcal{O}(n_{\boldsymbol{u}})$ operations are required to evaluate

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

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

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

and **hyperreduced** model[3] is independent of $n_{\boldsymbol{u}}$



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

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

Trust region ingredients for global convergence

Approximation models

$$m_k(\boldsymbol{\mu}),\ \psi_k(\boldsymbol{\mu})$$

Error indicators

$$\begin{aligned}
|F(\boldsymbol{\mu}_k) - F(\boldsymbol{\mu}) + m_k(\boldsymbol{\mu}) - m_k(\boldsymbol{\mu}_k)| &\leq \zeta \vartheta_k(\boldsymbol{\mu}) & \zeta > 0 \\
||\nabla F(\boldsymbol{\mu}) - \nabla m_k(\boldsymbol{\mu})|| &\leq \xi \varphi_k(\boldsymbol{\mu}) & \xi > 0 \\
|F(\boldsymbol{\mu}_k) - F(\boldsymbol{\mu}) + \psi_k(\boldsymbol{\mu}) - \psi_k(\boldsymbol{\mu}_k)| &\leq \sigma \theta_k(\boldsymbol{\mu}) & \sigma > 0
\end{aligned}$$

Adaptivity

$$\begin{aligned}
\vartheta_k(\boldsymbol{\mu}_k) &\leq \kappa_\vartheta \Delta_k \\
\varphi_k(\boldsymbol{\mu}_k) &\leq \kappa_\varphi \min\{||\nabla m_k(\boldsymbol{\mu}_k)||\,,\ \Delta_k\} \\
\theta_k(\hat{\boldsymbol{\mu}}_k)^\omega &\leq \eta \min\{m_k(\boldsymbol{\mu}_k) - m_k(\hat{\boldsymbol{\mu}}_k),\ r_k\}
\end{aligned}$$

Global convergence

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

Trust region method: ROM approximation model

Approximation models based on reduced-order models

$$m_k(\boldsymbol{\mu}) = \mathcal{J}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu}) \qquad \psi_k(\boldsymbol{\mu}) = \mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu}),\, \boldsymbol{\mu})$$

Error indicators from residual-based error bounds

$$\begin{aligned}
\vartheta_k(\boldsymbol{\mu}) &= ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}_k),\, \boldsymbol{\mu}_k)||_{\boldsymbol{\Theta}} + ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})||_{\boldsymbol{\Theta}} \\
\varphi_k(\boldsymbol{\mu}) &= ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})||_{\boldsymbol{\Theta}} + \left|\left|\boldsymbol{r}^{\boldsymbol{\lambda}}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\Psi}_k \boldsymbol{\lambda}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})\right|\right|_{\boldsymbol{\Theta}^{\boldsymbol{\lambda}}} \\
\theta_k(\boldsymbol{\mu}) &= 0
\end{aligned}$$

Adaptivity to refine basis at trust region center

$$\boldsymbol{\Phi}_k = \begin{bmatrix} \boldsymbol{u}(\boldsymbol{\mu}_k) & \boldsymbol{\lambda}(\boldsymbol{\mu}_k) & \texttt{POD}(\boldsymbol{U}_k) & \texttt{POD}(\boldsymbol{V}_k) \end{bmatrix}$$

$$\boldsymbol{U}_k = \begin{bmatrix} \boldsymbol{u}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{u}(\boldsymbol{\mu}_{k-1}) \end{bmatrix} \qquad \boldsymbol{V}_k = \begin{bmatrix} \boldsymbol{\lambda}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{\lambda}(\boldsymbol{\mu}_{k-1}) \end{bmatrix}$$

$$\text{Interpolation property} \implies \vartheta_k(\boldsymbol{\mu}_k) = \varphi_k(\boldsymbol{\mu}_k) = 0$$

Approximation models based on reduced-order models

$$m_k(\boldsymbol{\mu}) = \mathcal{J}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu}) \qquad \psi_k(\boldsymbol{\mu}) = \mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu}),\, \boldsymbol{\mu})$$

Error indicators from residual-based error bounds

$$\begin{aligned}
\vartheta_k(\boldsymbol{\mu}) &= ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}_k),\, \boldsymbol{\mu}_k)||_{\boldsymbol{\Theta}} + ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})||_{\boldsymbol{\Theta}} \\
\varphi_k(\boldsymbol{\mu}) &= ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})||_{\boldsymbol{\Theta}} + \left|\left|\boldsymbol{r}^{\boldsymbol{\lambda}}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\Psi}_k \boldsymbol{\lambda}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})\right|\right|_{\boldsymbol{\Theta}^{\boldsymbol{\lambda}}} \\
\theta_k(\boldsymbol{\mu}) &= 0
\end{aligned}$$

Adaptivity to refine basis at trust region center

$$\boldsymbol{\Phi}_k = \begin{bmatrix} \boldsymbol{u}(\boldsymbol{\mu}_k) & \boldsymbol{\lambda}(\boldsymbol{\mu}_k) & \mathtt{POD}(\boldsymbol{U}_k) & \mathtt{POD}(\boldsymbol{V}_k) \end{bmatrix}$$

$$\boldsymbol{U}_k = \begin{bmatrix} \boldsymbol{u}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{u}(\boldsymbol{\mu}_{k-1}) \end{bmatrix} \qquad \boldsymbol{V}_k = \begin{bmatrix} \boldsymbol{\lambda}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{\lambda}(\boldsymbol{\mu}_{k-1}) \end{bmatrix}$$

$$\text{Interpolation property} \implies \vartheta_k(\boldsymbol{\mu}_k) = \varphi_k(\boldsymbol{\mu}_k) = 0$$

$$\liminf_{k\to\infty} \; ||\nabla \mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu}_k),\, \boldsymbol{\mu}_k)|| = 0$$

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

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

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*

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

Source of inexactness: **Partially Converged Solution (PCS)**

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

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

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

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

Trust region method: ROM/PCS approximation model

Approximation models based on ROMs and partially converged solutions

$$m_k(\boldsymbol{\mu}) = \mathcal{J}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu}) \qquad \psi_k(\boldsymbol{\mu}) = \mathcal{J}(\boldsymbol{u}^{\tau_k}(\boldsymbol{\mu}),\, \boldsymbol{\mu})$$

Error indicators from residual-based error bounds

$$\vartheta_k(\boldsymbol{\mu}) = \left|\left|\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}_k),\, \boldsymbol{\mu}_k)\right|\right|_{\boldsymbol{\Theta}} + \left|\left|\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})\right|\right|_{\boldsymbol{\Theta}}$$
$$\varphi_k(\boldsymbol{\mu}) = \left|\left|\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})\right|\right|_{\boldsymbol{\Theta}} + \left|\left|\boldsymbol{r}^{\boldsymbol{\lambda}}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\Psi}_k \boldsymbol{\lambda}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})\right|\right|_{\boldsymbol{\Theta}^{\boldsymbol{\lambda}}}$$
$$\theta_k(\boldsymbol{\mu}) = \left|\left|\boldsymbol{r}(\boldsymbol{u}^{\tau_k}(\boldsymbol{\mu}_k),\, \boldsymbol{\mu}_k)\right|\right|_{\boldsymbol{\Theta}} + \left|\left|\boldsymbol{r}(\boldsymbol{u}^{\tau_k}(\boldsymbol{\mu}),\, \boldsymbol{\mu})\right|\right|_{\boldsymbol{\Theta}}$$

Adaptivity to refine basis at trust region center

$$\boldsymbol{\Phi}_k = \begin{bmatrix} \boldsymbol{u}^{\alpha_k}(\boldsymbol{\mu}_k) & \boldsymbol{\lambda}^{\alpha_k,\,\beta_k}(\boldsymbol{\mu}_k) & \texttt{POD}(\boldsymbol{U}_k) & \texttt{POD}(\boldsymbol{V}_k) \end{bmatrix}$$
$$\boldsymbol{U}_k = \begin{bmatrix} \boldsymbol{u}^{\alpha_0}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{u}^{\alpha_{k-1}}(\boldsymbol{\mu}_{k-1}) \end{bmatrix} \qquad \boldsymbol{V}_k = \begin{bmatrix} \boldsymbol{\lambda}^{\alpha_0,\,\beta_0}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{\lambda}^{\alpha_{k-1},\,\beta_{k-1}}(\boldsymbol{\mu}_{k-1}) \end{bmatrix}$$

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

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

Trust region method: ROM/PCS approximation model

Approximation models based on ROMs and partially converged solutions

$$m_k(\boldsymbol{\mu}) = \mathcal{J}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu}) \qquad \psi_k(\boldsymbol{\mu}) = \mathcal{J}(\boldsymbol{u}^{\tau_k}(\boldsymbol{\mu}),\, \boldsymbol{\mu})$$

Error indicators from residual-based error bounds

$$\vartheta_k(\boldsymbol{\mu}) = ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}_k),\, \boldsymbol{\mu}_k)||_{\boldsymbol{\Theta}} + ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})||_{\boldsymbol{\Theta}}$$
$$\varphi_k(\boldsymbol{\mu}) = ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})||_{\boldsymbol{\Theta}} + \left|\left|\boldsymbol{r}^{\boldsymbol{\lambda}}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\Psi}_k \boldsymbol{\lambda}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})\right|\right|_{\boldsymbol{\Theta}^{\boldsymbol{\lambda}}}$$
$$\theta_k(\boldsymbol{\mu}) = ||\boldsymbol{r}(\boldsymbol{u}^{\tau_k}(\boldsymbol{\mu}_k),\, \boldsymbol{\mu}_k)||_{\boldsymbol{\Theta}} + ||\boldsymbol{r}(\boldsymbol{u}^{\tau_k}(\boldsymbol{\mu}),\, \boldsymbol{\mu})||_{\boldsymbol{\Theta}}$$

Adaptivity to refine basis at trust region center

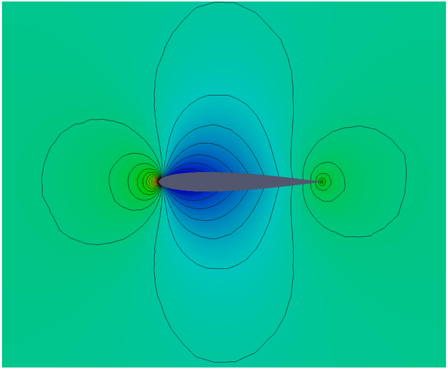
$$\boldsymbol{\Phi}_k = \begin{bmatrix} \boldsymbol{u}^{\alpha_k}(\boldsymbol{\mu}_k) & \boldsymbol{\lambda}^{\alpha_k,\,\beta_k}(\boldsymbol{\mu}_k) & \texttt{POD}(\boldsymbol{U}_k) & \texttt{POD}(\boldsymbol{V}_k) \end{bmatrix}$$
$$\boldsymbol{U}_k = \begin{bmatrix} \boldsymbol{u}^{\alpha_0}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{u}^{\alpha_{k-1}}(\boldsymbol{\mu}_{k-1}) \end{bmatrix} \qquad \boldsymbol{V}_k = \begin{bmatrix} \boldsymbol{\lambda}^{\alpha_0,\,\beta_0}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{\lambda}^{\alpha_{k-1},\,\beta_{k-1}}(\boldsymbol{\mu}_{k-1}) \end{bmatrix}$$

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

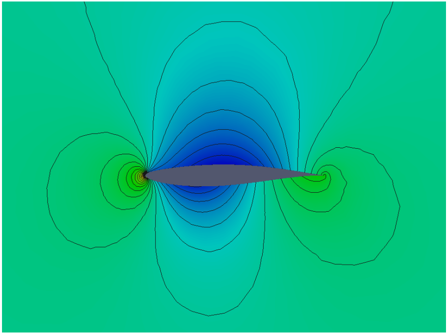
$$\vartheta_k(\boldsymbol{\mu}_k) \leq \kappa_\vartheta \Delta_k \qquad \varphi_k(\boldsymbol{\mu}_k) \leq \kappa_\varphi \min\{||\nabla m_k(\boldsymbol{\mu}_k)||\,,\, \Delta_k\}$$
$$\theta_k^\omega(\hat{\boldsymbol{\mu}}_k) \leq \eta \min\{m_k(\boldsymbol{\mu}_k) - m_k(\hat{\boldsymbol{\mu}}_k),\, r_k\}$$

$$\liminf_{k\to\infty} \; ||\nabla \mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu}_k),\, \boldsymbol{\mu}_k)|| = 0$$

Pressure discrepancy minimization (Euler equations)



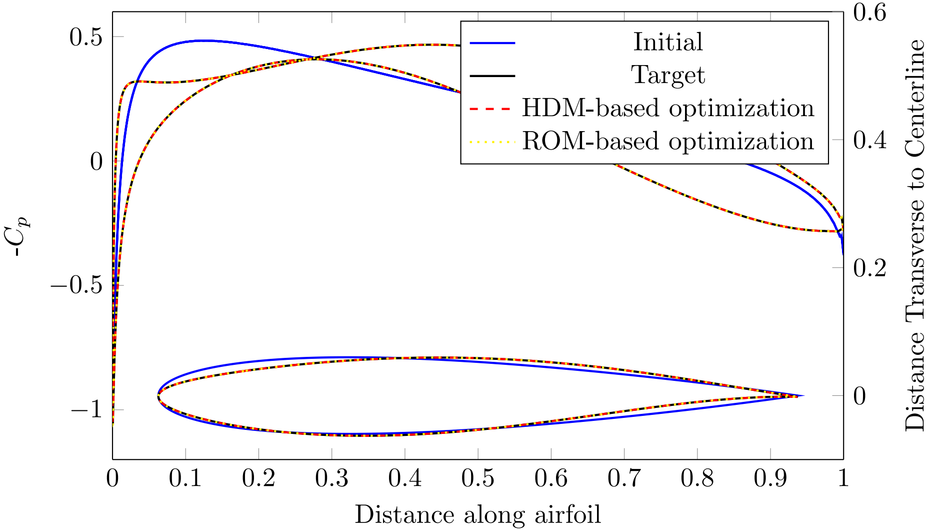
NACA0012: Initial



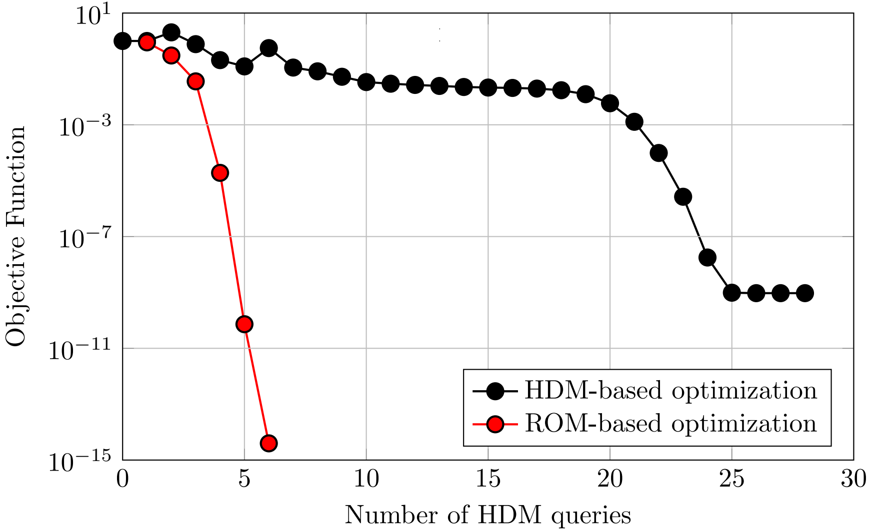
RAE2822: Target

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

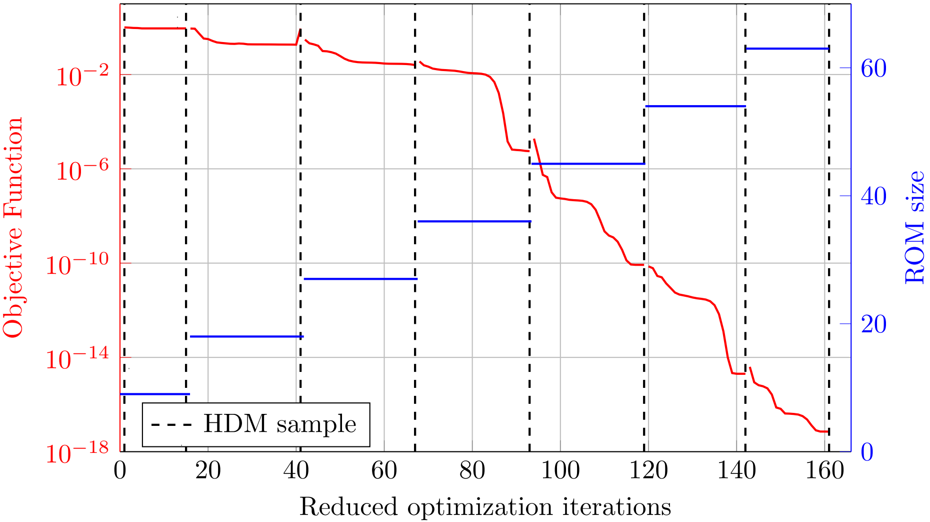
Proposed method: recovers target airfoil



Proposed method: 4× fewer HDM queries



At the cost of ROM queries

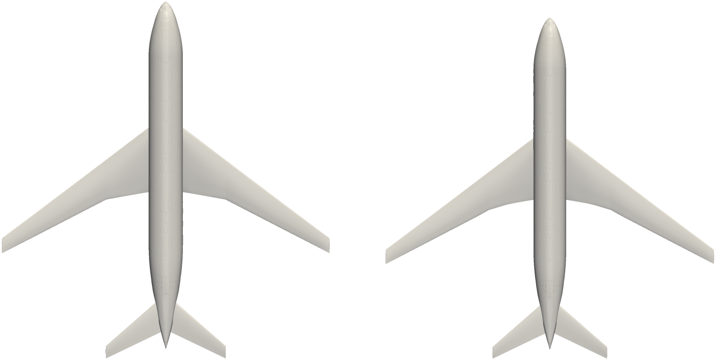


Shape optimization of aircraft in turbulent flow

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

- **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

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



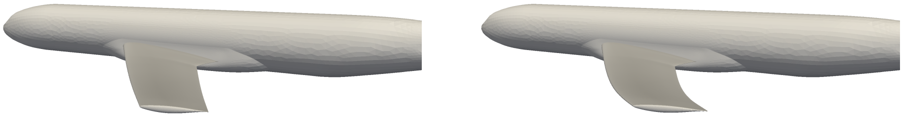
Wingspan

Shape optimization of aircraft in turbulent flow

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

- **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

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



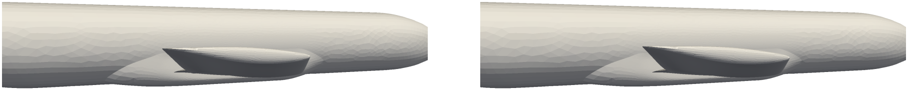
Localized sweep

Shape optimization of aircraft in turbulent flow

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

- **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

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



Twist

Shape optimization of aircraft in turbulent flow

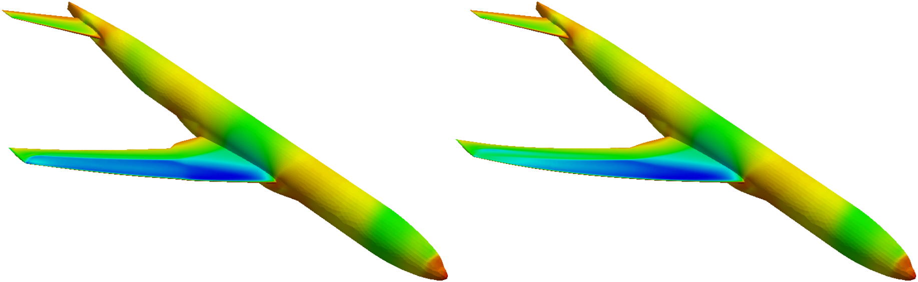
$$\begin{aligned} \underset{\boldsymbol{\mu} \in \mathbb{R}^4}{\text{minimize}} \quad & -L_z(\boldsymbol{\mu})/L_x(\boldsymbol{\mu}) \\ \text{subject to} \quad & L_z(\boldsymbol{\mu}) = \bar{L}_z \end{aligned}$$

- **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

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

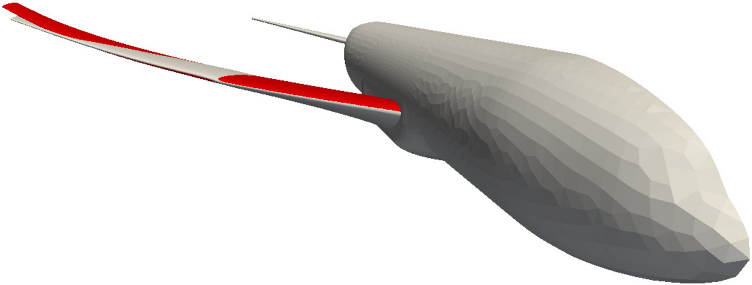
Localized dihedral

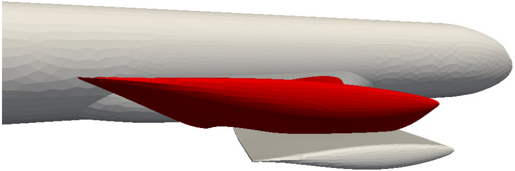
Optimized shape: reduction in **2.2** drag counts



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

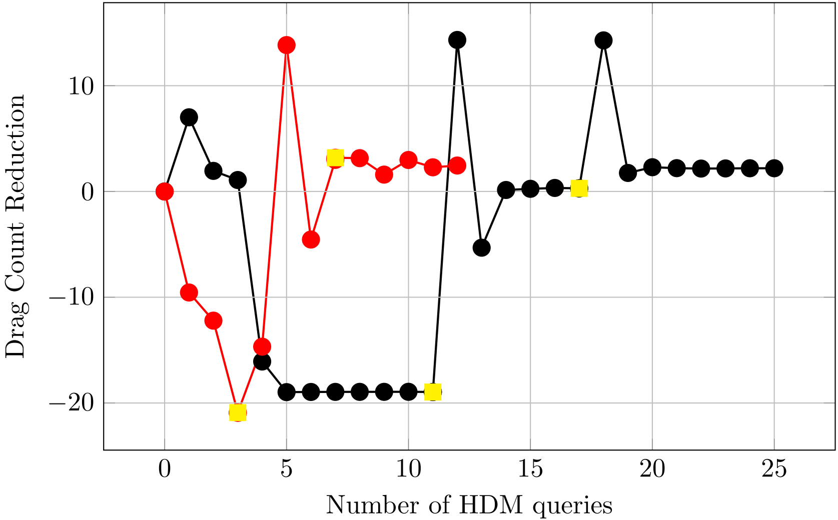
Optimized shape: reduction in **2.2** drag counts





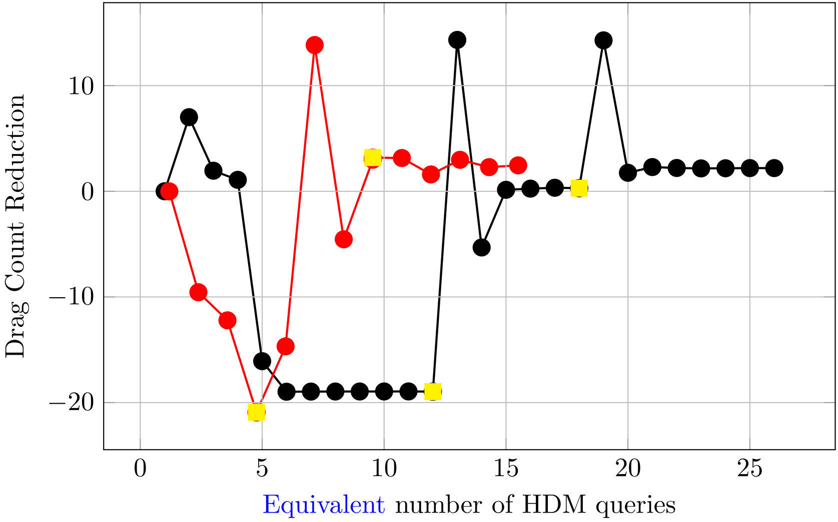
Baseline (gray) and optimized shape (red) – 2× magnification

Proposed method: **2x** reduction in number of HDM queries



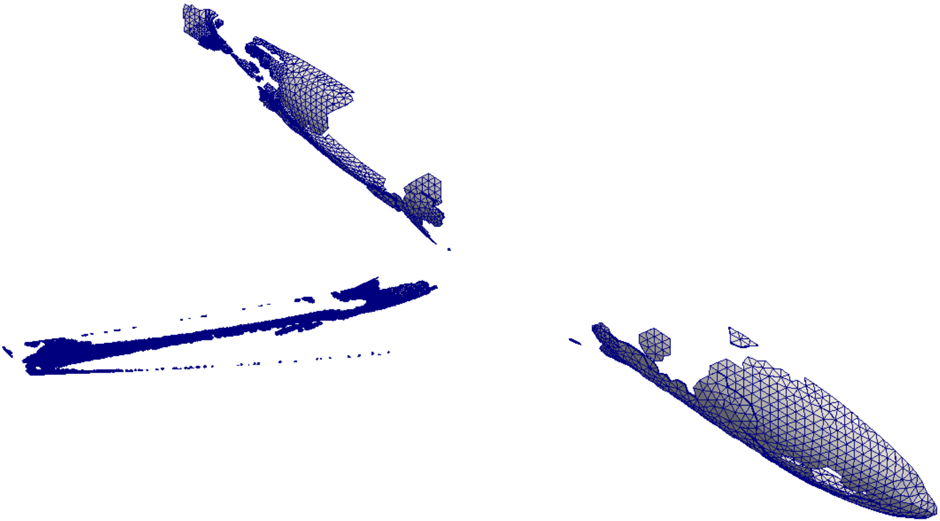
(—●—) HDM optimization, (—●—) ROM optimization,
(■) Augmented Lagrangian update

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

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

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

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

$$\Downarrow$$

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

[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

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

$$\Downarrow$$

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

$$\Downarrow$$

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

Proposed approach: managed inexactness

Replace expensive PDE with inexpensive approximation model

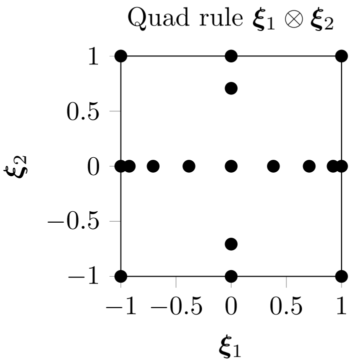
- **Reduced-order models** used for *inexact PDE evaluations*
- **Partially converged solutions** used for *inexact PDE evaluations*
- **Anisotropic sparse grids** used for *inexact integration* of risk measures

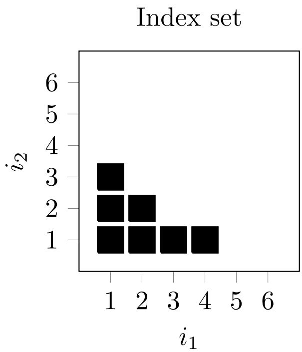
$$\underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad F(\boldsymbol{\mu}) \qquad \longrightarrow \qquad \underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad m_k(\boldsymbol{\mu})$$

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*

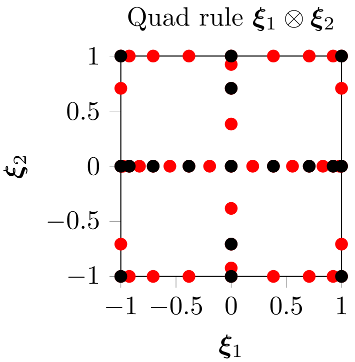
$$\underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad F(\boldsymbol{\mu}) \qquad \longrightarrow \qquad \begin{aligned} &\underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} && m_k(\boldsymbol{\mu}) \\ &\text{subject to} && ||\boldsymbol{\mu}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

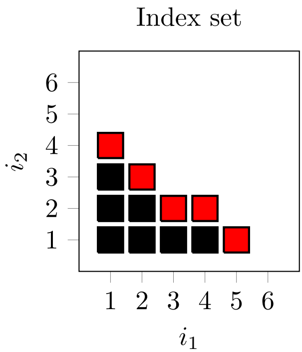




Index set ($\mathcal{I}$) – ● Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

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

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

Error indicators that account for both sources of error

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

Reduced-order model errors

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

Sparse grid truncation errors

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

Final requirement for convergence: **Adaptivity**

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

$$m_k(\boldsymbol{\mu}) = \mathbb{E}_{\mathcal{I}_k}\left[\mathcal{J}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu},\,\cdot\,),\, \boldsymbol{\mu},\,\cdot\,)\right]$$
$$\varphi_k(\boldsymbol{\mu}) = \alpha_1 \mathcal{E}_1(\boldsymbol{\mu};\, \mathcal{I}_k,\, \boldsymbol{\Phi}_k) + \alpha_2 \mathcal{E}_2(\boldsymbol{\mu};\, \mathcal{I}_k,\, \boldsymbol{\Phi}_k) + \alpha_3 \mathcal{E}_4(\boldsymbol{\mu};\, \mathcal{I}_k,\, \boldsymbol{\Phi}_k)$$

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

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

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

$$\mathcal{E}_1(\boldsymbol{\mu}_k;\, \mathcal{I},\, \boldsymbol{\Phi}) \leq \frac{\kappa_\varphi}{3\alpha_1} \min\{||\nabla m_k(\boldsymbol{\mu}_k)||\,,\, \Delta_k\}$$
$$\mathcal{E}_2(\boldsymbol{\mu}_k;\, \mathcal{I},\, \boldsymbol{\Phi}) \leq \frac{\kappa_\varphi}{3\alpha_2} \min\{||\nabla m_k(\boldsymbol{\mu}_k)||\,,\, \Delta_k\}$$
$$\mathcal{E}_4(\boldsymbol{\mu}_k;\, \mathcal{I},\, \boldsymbol{\Phi}) \leq \frac{\kappa_\varphi}{3\alpha_3} \min\{||\nabla m_k(\boldsymbol{\mu}_k)||\,,\, \Delta_k\}$$

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

Refine index set: Dimension-adaptive sparse grids

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

Adaptivity: Dimension-adaptive greedy method

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

Refine index set: Dimension-adaptive sparse grids

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

Refine reduced-order basis: Greedy sampling

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

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

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

end while

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

Refine index set: Dimension-adaptive sparse grids

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end while

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

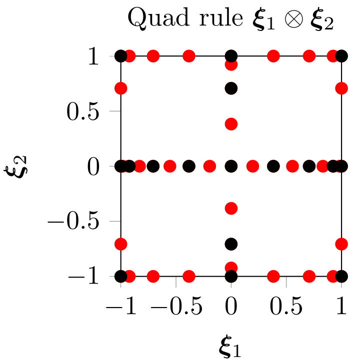
$$\mathbf{\Phi}_k \leftarrow \begin{bmatrix}\mathbf{\Phi}_k & \boldsymbol{u}(\boldsymbol{\mu}_k, \boldsymbol{\xi}^*) & \boldsymbol{\lambda}(\boldsymbol{\mu}_k, \boldsymbol{\xi}^*)\end{bmatrix}$$

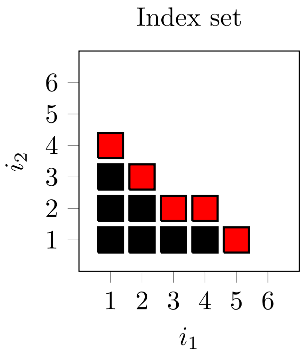
$$\boldsymbol{\xi}^* = \underset{\boldsymbol{\xi}\in\mathbf{\Xi}_{\mathbf{j}^*}}{\arg\max}\ \rho(\boldsymbol{\xi})\left|\left|\boldsymbol{r}^{\boldsymbol{\lambda}}(\mathbf{\Phi}_k\boldsymbol{u}_r(\boldsymbol{\mu}_k, \boldsymbol{\xi}), \mathbf{\Psi}_k\boldsymbol{\lambda}_r(\boldsymbol{\mu}_k, \boldsymbol{\xi}),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

end while

end while

Anisotropic sparse grid quadrature: neighbors





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

Optimal control of steady Burgers' equation

- **Optimization problem:**

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

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

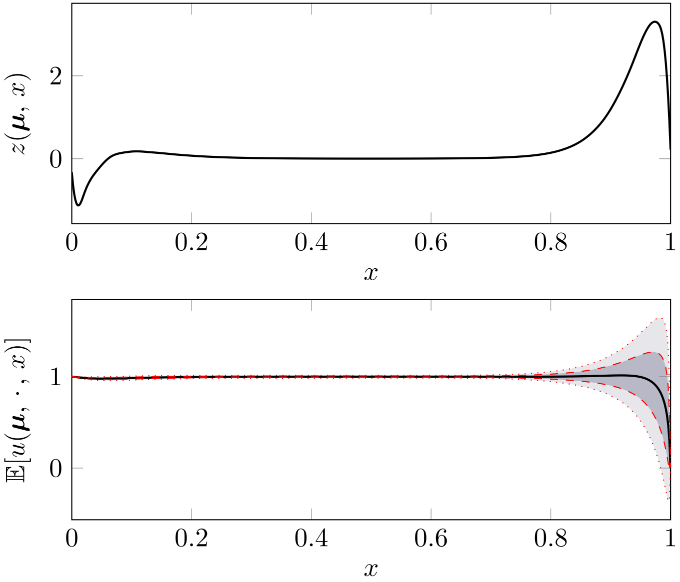
$$-\nu(\boldsymbol{\xi})\partial_{xx}u(\boldsymbol{\mu}, \boldsymbol{\xi}, x) + u(\boldsymbol{\mu}, \boldsymbol{\xi}, x)\partial_x u(\boldsymbol{\mu}, \boldsymbol{\xi}, x) = z(\boldsymbol{\mu}, x) \quad x \in (0, 1), \quad \boldsymbol{\xi} \in \boldsymbol{\Xi}$$
$$u(\boldsymbol{\mu}, \boldsymbol{\xi},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

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

$$\nu(\boldsymbol{\xi}) = 10^{\boldsymbol{\xi}_1 - 2} \qquad d_0(\boldsymbol{\xi}) = 1 + \frac{\boldsymbol{\xi}_2}{1000} \qquad d_1(\boldsymbol{\xi}) = \frac{\boldsymbol{\xi}_3}{1000}$$

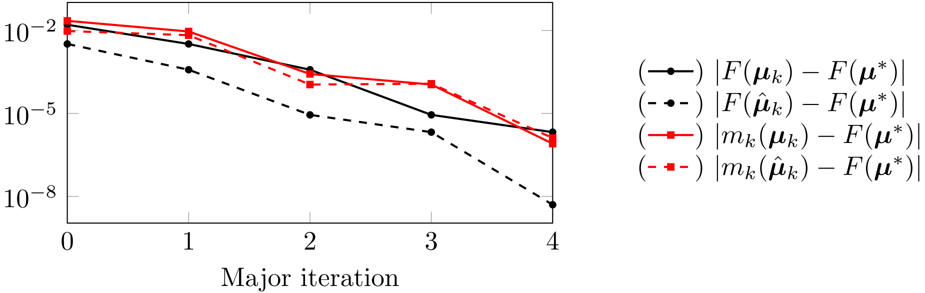
- **Parametrization:** $z(\boldsymbol{\mu}, x)$ – cubic splines with 51 knots, $n_{\boldsymbol{\mu}} = 53$

Optimal control and statistics



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

Global convergence without pointwise agreement

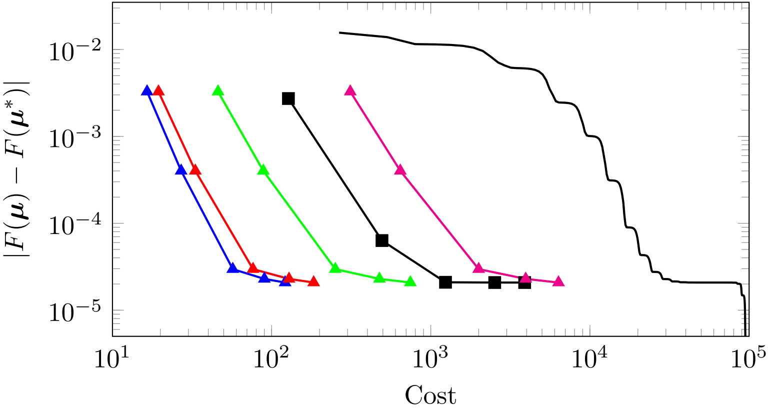


$F(\boldsymbol{\mu}_k)$	$m_k(\boldsymbol{\mu}_k)$	$F(\hat{\boldsymbol{\mu}}_k)$	$m_k(\hat{\boldsymbol{\mu}}_k)$	$\|\|\nabla F(\boldsymbol{\mu}_k)\|\|$	ρ_k	Success?
6.6506e-02	7.2694e-02	5.3655e-02	5.9922e-02	2.2959e-02	1.0257e+00	1.0000e+00
5.3655e-02	5.9593e-02	5.0783e-02	5.7152e-02	2.3424e-03	9.7512e-01	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

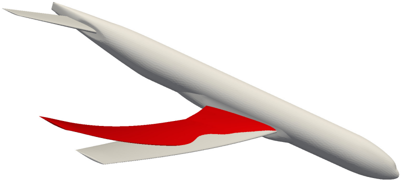
Significant reduction in cost, even if (largest) ROM only 10× faster than HDM

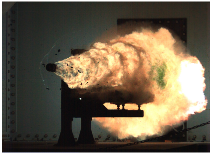
$$\text{Cost} = \text{nHdmPrim} + 0.5 \times \text{nHdmAdj} + \tau^{-1} \times (\text{nRomPrim} + 0.5 \times \text{nRomAdj})$$

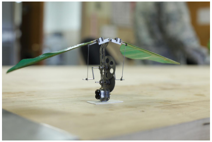


5-level isotropic SG (—), dimension-adaptive SG [Kouri et al., 2014] (-■-), and proposed ROM/SG for $\tau = 1$ (-▲-), $\tau = 10$ (-▲-), $\tau = 100$ (-▲-), $\tau = \infty$ (-▲-)

- 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

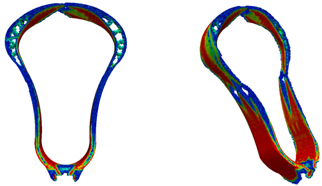


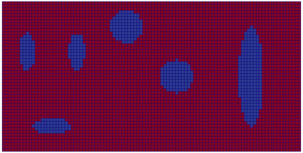


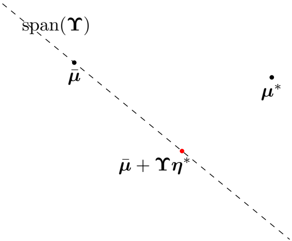


Extension to problems with **many parameters**

- Topology optimization[4] and inverse problems
- **Nested reduction** of state and parameter
- Multifidelity trust region method to globalize **state** reduction
- Linesearch/subspace method to globalize **parameter** reduction

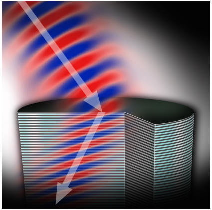


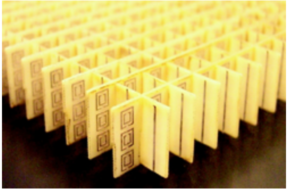




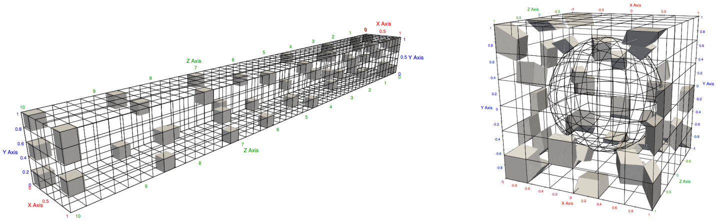
[4]Increasingly relevant due to emergence of Additive Manufacturing – ***MIT Technology Review*, Top 10 Technological Breakthrough 2013**

Extension to **multiscale** problems





- **Existing multiscale methods** are extremely expensive
  - Single simulation: 203 hours ($\approx$ 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*



Hyperreduced model for macroscale (left) and microstructure (right)

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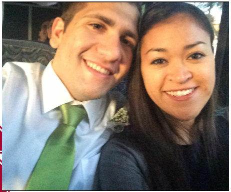

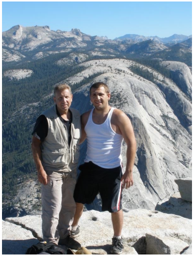

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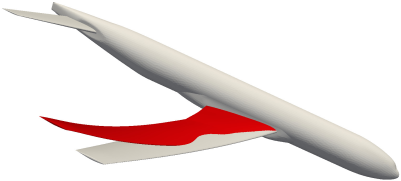

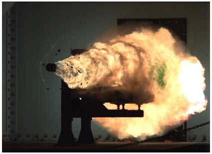

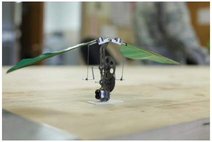

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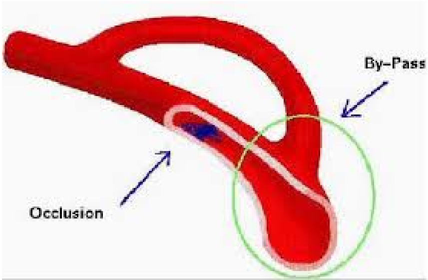
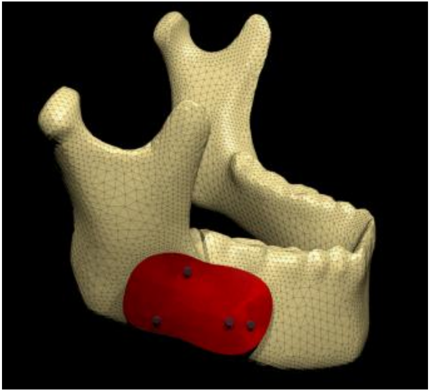
Computers and Fluids.

PDE optimization is **ubiquitous** in science and engineering

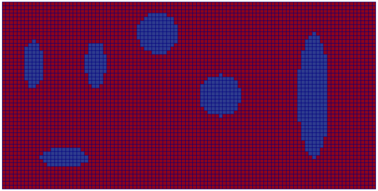
Design: Find system that optimizes performance metric, satisfies constraints

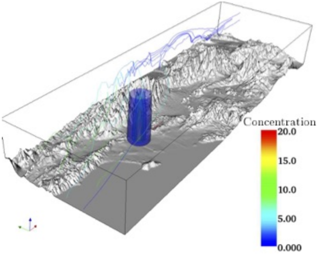




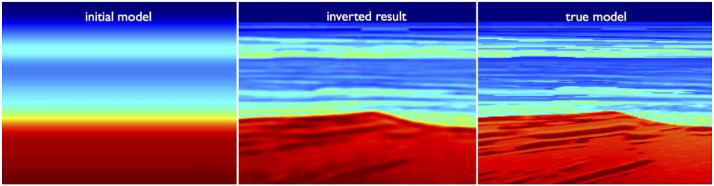
Shape design of arterial bypass (left) and shape/topology design of patient-specific implant (right)

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 measurements

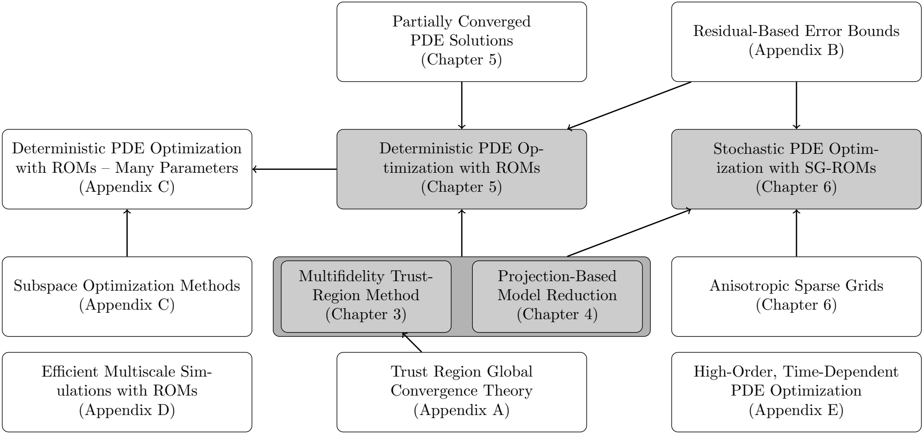
Applications in computational mechanics: dynamic

Energy = 9.4096e+00	Energy = 4.9476e+00	Energy = 4.6110e+00
Thrust = 1.7660e-01	Thrust = 2.5000e+00	Thrust = 2.5000e+00

Initial	Optimal Control	Optimal Shape/Control

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

Thesis organization



Overview of global convergence theory[5]

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

Lemma 1: $\Delta_k \to 0$

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

Lemma 2: $\rho_k \to 1$

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

Theorem 1: $\liminf ||\nabla F(\boldsymbol{\mu}_k)|| = 0$

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

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

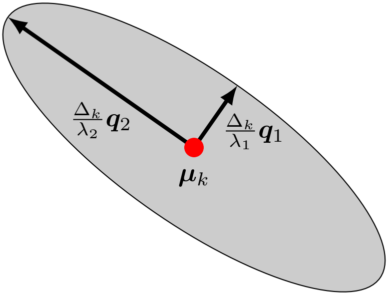
An interpretation of **error-aware** trust regions

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

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

Then, to first order[6],

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



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

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

Optimization of the Rosenbrock function

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

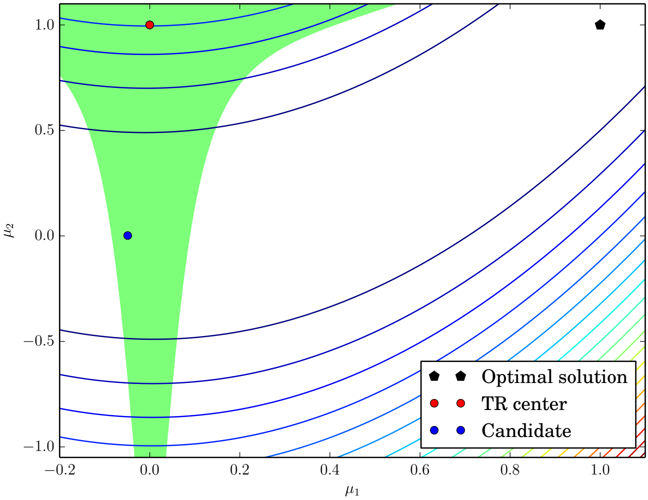
using the approximation models and error indicators

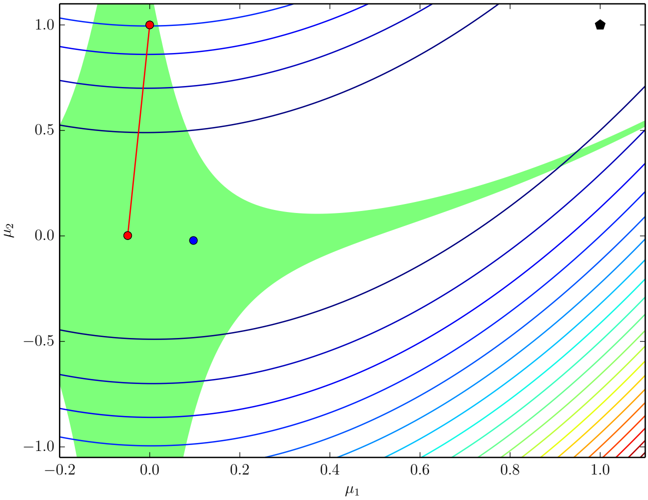
$$\begin{aligned}
m_k(\boldsymbol{\mu}) &\equiv G_k(\boldsymbol{\mu};\ \epsilon_k,\ \delta_k)\\
\psi_k(\boldsymbol{\mu}) &\equiv F(\boldsymbol{\mu})\\
\vartheta_k(\boldsymbol{\mu}) &\equiv |F(\boldsymbol{\mu}) - G_k(\boldsymbol{\mu};\, \epsilon_k,\, \delta_k)| + |F(\boldsymbol{\mu}_k) - G_k(\boldsymbol{\mu}_k;\,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

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

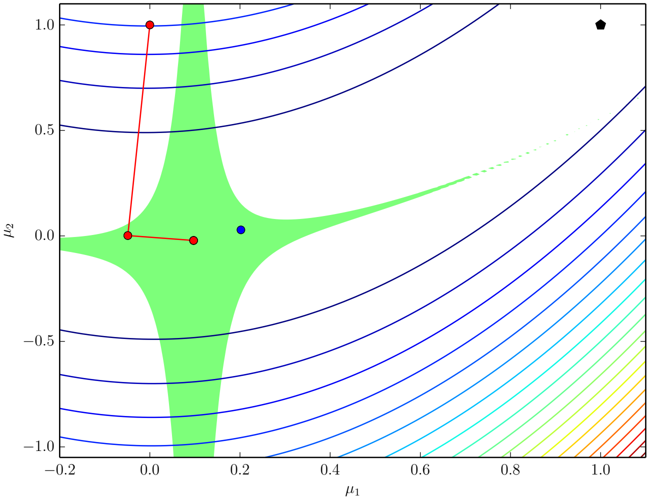
$$G_k(\boldsymbol{\mu};\, \epsilon,\, \delta) \equiv F(\boldsymbol{\mu}_k) + \epsilon + (\nabla F(\boldsymbol{\mu}_k) + \delta\mathbf{1})^T(\boldsymbol{\mu} - \boldsymbol{\mu}_k) + \frac{1}{2}(\boldsymbol{\mu} - \boldsymbol{\mu}_k)^T \nabla^2 F(\boldsymbol{\mu}_k)(\boldsymbol{\mu} - \boldsymbol{\mu}_k)$$

A look at **error-aware** trust regions

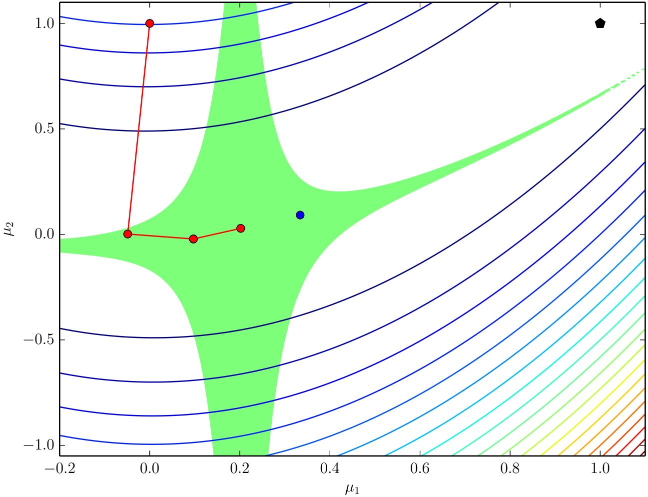



1.0
0.5
0.0
−0.5
−1.0
μ_2
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
μ_1

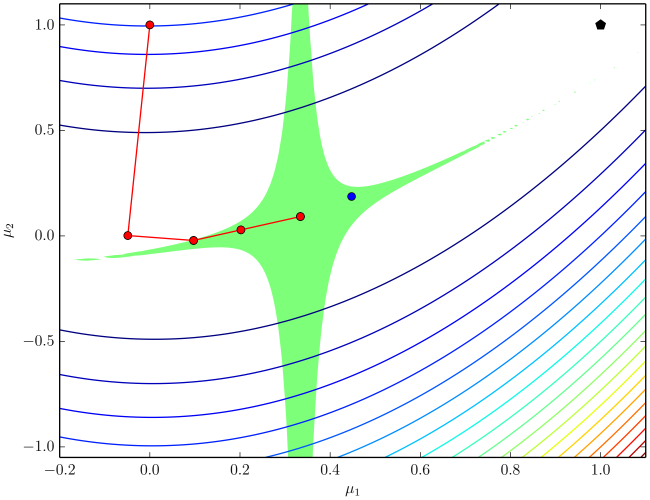
A look at **error-aware** trust regions



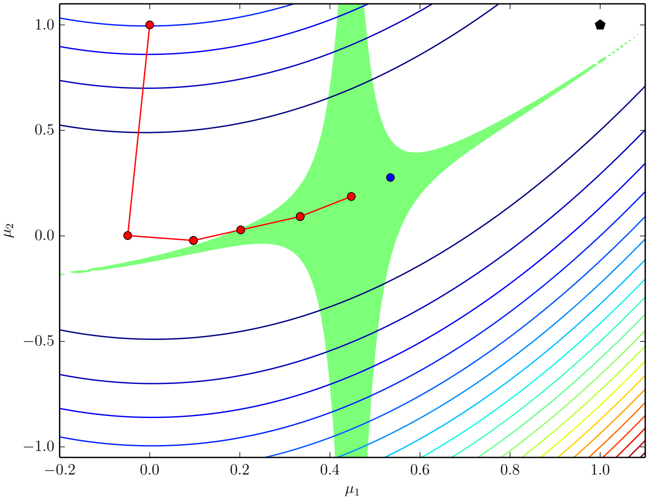
A look at **error-aware** trust regions



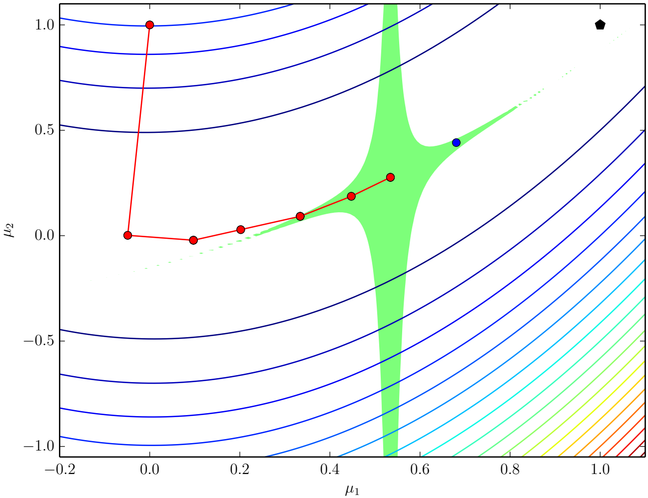
A look at **error-aware** trust regions



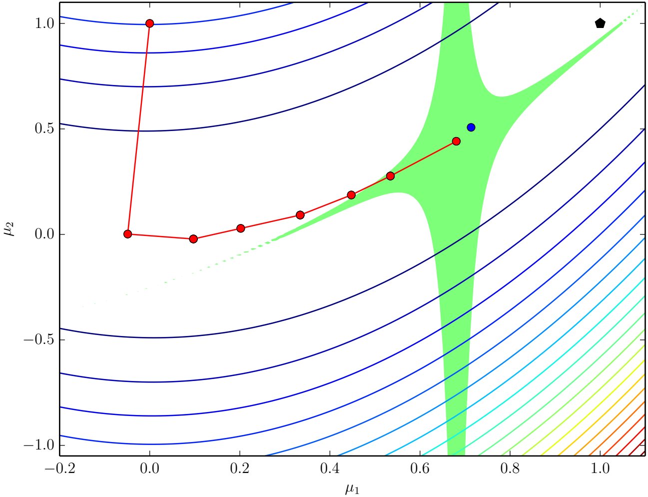
A look at **error-aware** trust regions



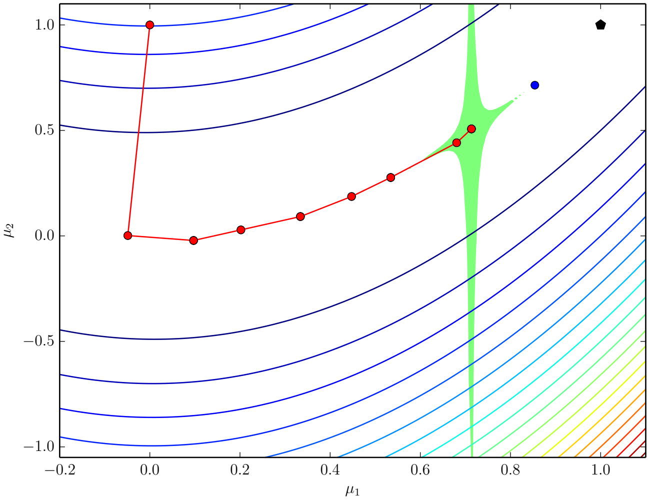
A look at **error-aware** trust regions



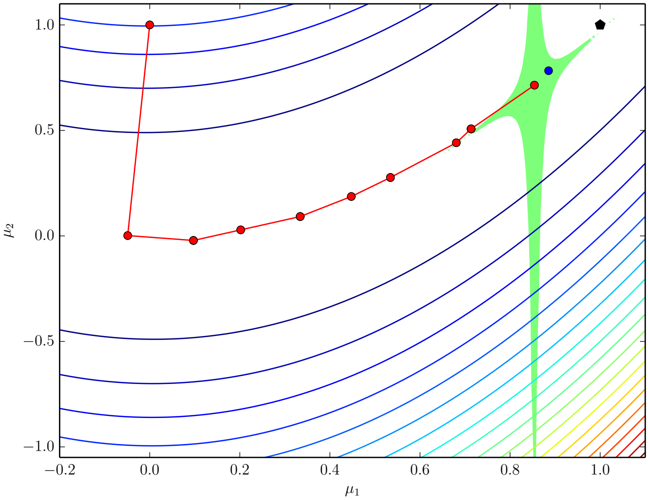
A look at **error-aware** trust regions



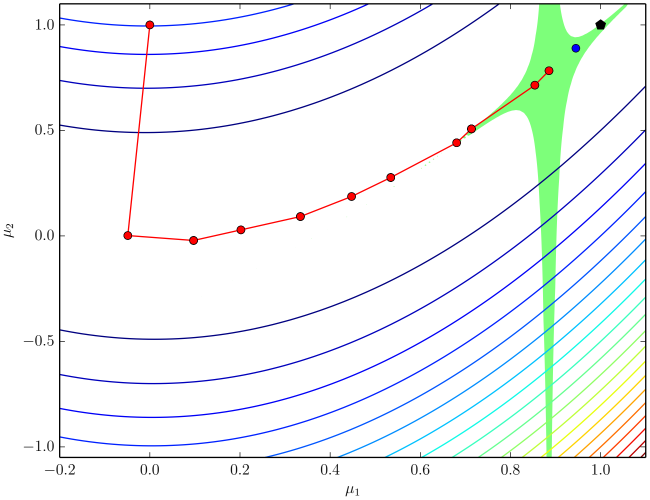
A look at **error-aware** trust regions



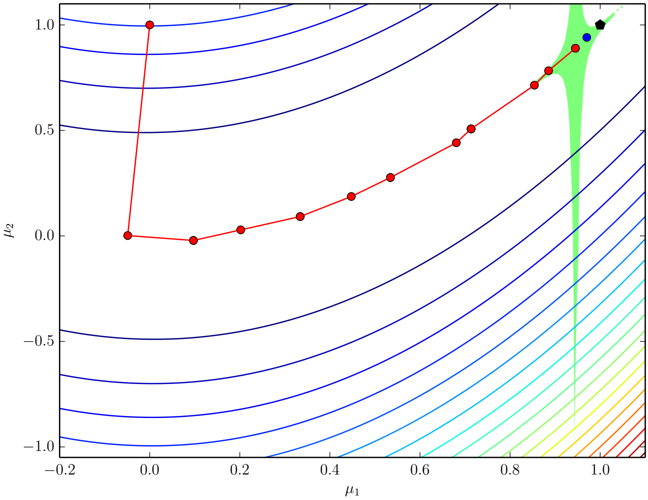
A look at **error-aware** trust regions



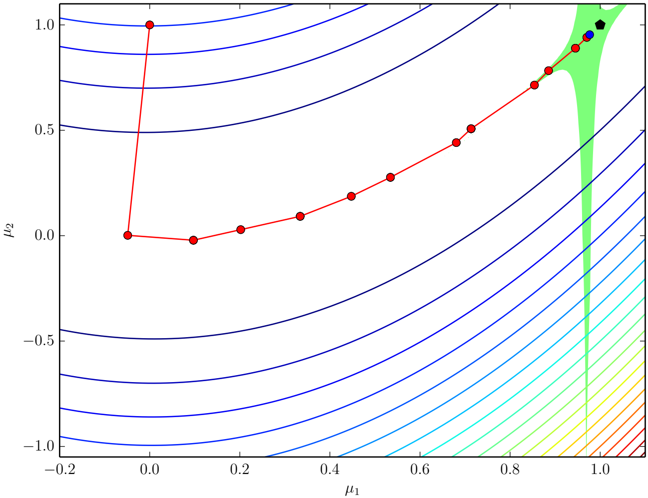
A look at **error-aware** trust regions



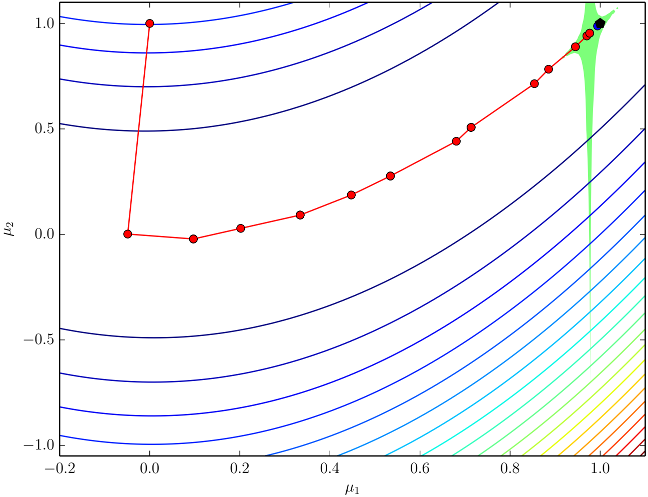
A look at **error-aware** trust regions



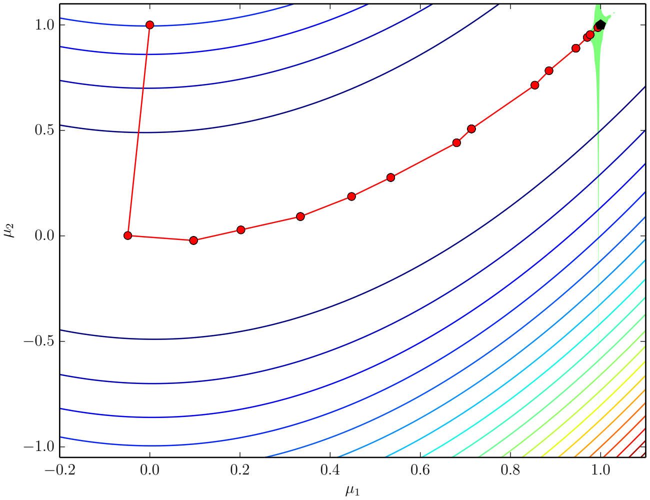
A look at **error-aware** trust regions



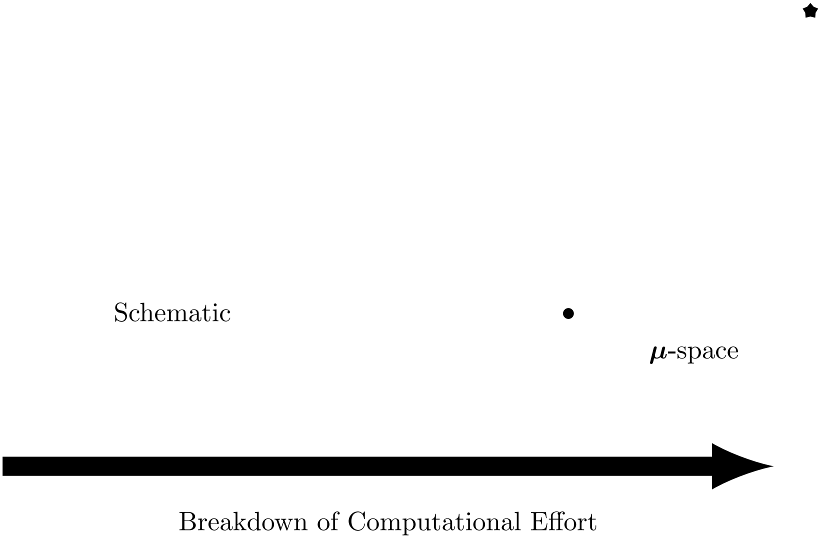
A look at **error-aware** trust regions

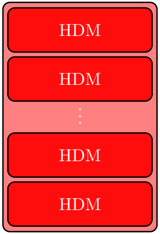


A look at **error-aware** trust regions

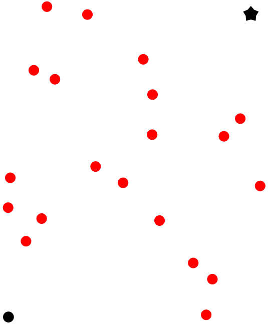


Offline-online approach to optimization with ROMs





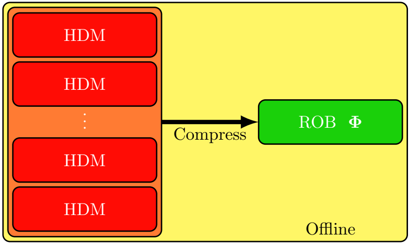
Schematic



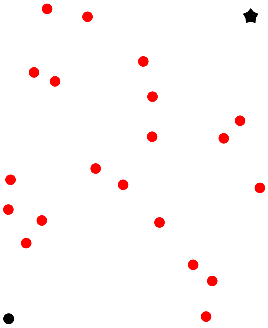
μ-space

Breakdown of Computational Effort

Offline-online approach to optimization with ROMs



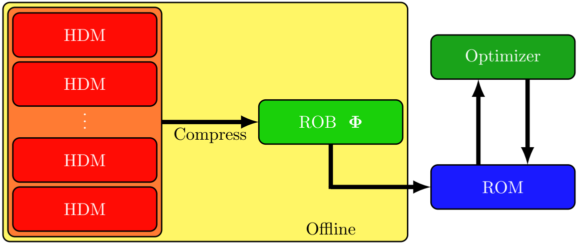
Schematic



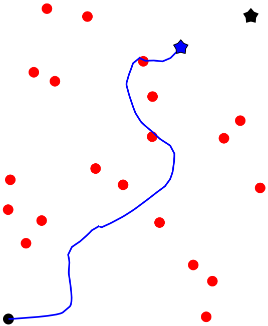
μ-space

Breakdown of Computational Effort

Offline-online approach to optimization with ROMs

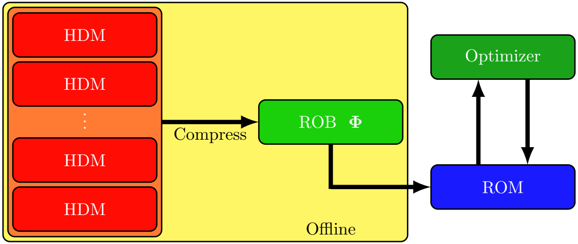


Schematic

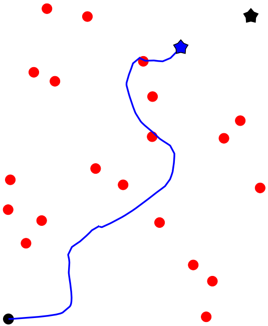


μ-space

Breakdown of Computational Effort



Schematic

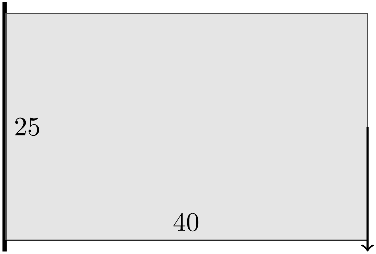


μ-space

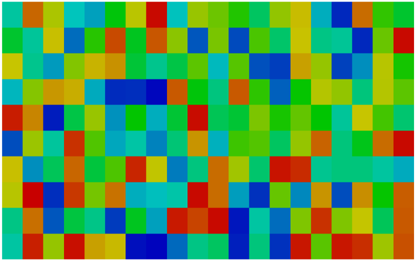
Breakdown of Computational Effort

No convergence **Scales exponentially with N_μ**

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

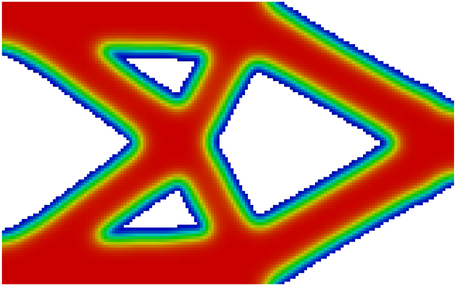


Stiffness maximization, volume constraint

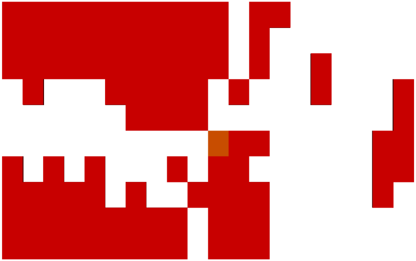


Parametrization with $n_{\boldsymbol{\mu}} = 200$

Numerical demonstration: offline-online breakdown



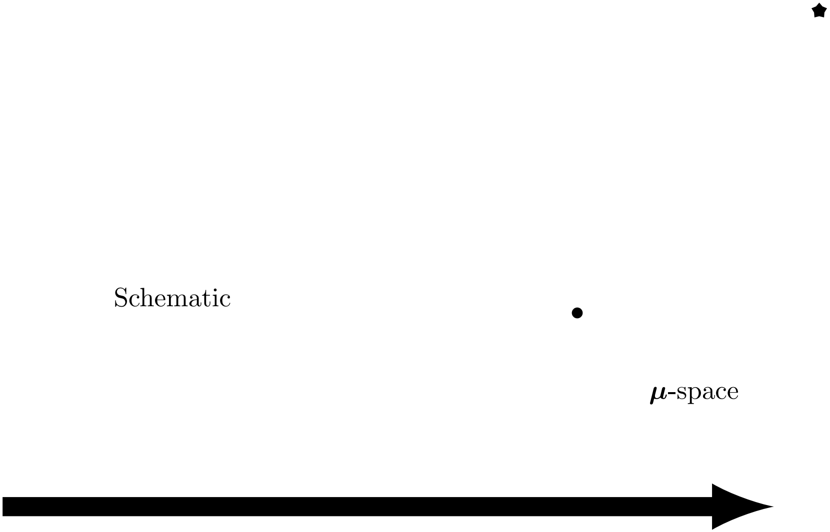
Optimal Solution
(1.97×10^4 s)



ROM Solution

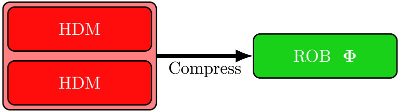
HDM Solution	**ROB** Construction	**Greedy** Algorithm	**ROM** Optimization
2.84×10^3 s	5.48×10^4 s	1.67×10^5 s	30 s
1.26%	24.36%	74.37%	0.01%

Schematic

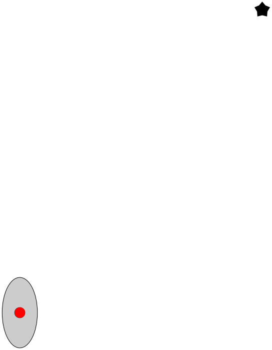


Breakdown of Computational Effort

Trust region framework for optimization with ROMs

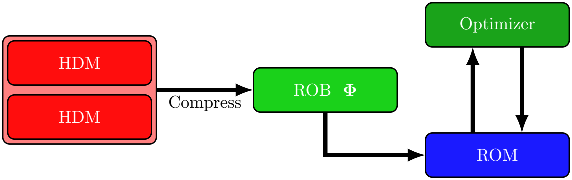


Schematic

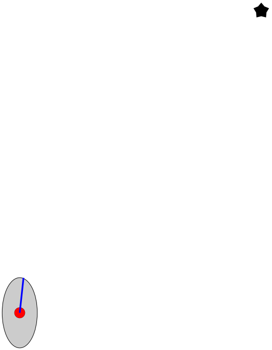


μ-space

Breakdown of Computational Effort



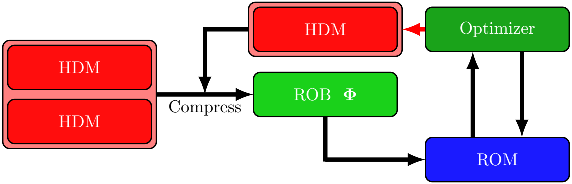
Schematic



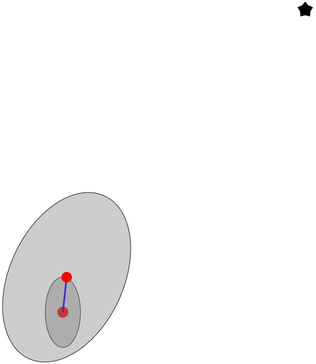
$\boldsymbol{\mu}$-space

Breakdown of Computational Effort

Trust region framework for optimization with ROMs

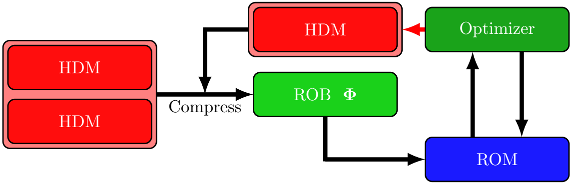


Schematic

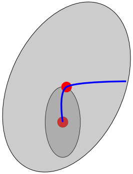


$\boldsymbol{\mu}$-space

Breakdown of Computational Effort

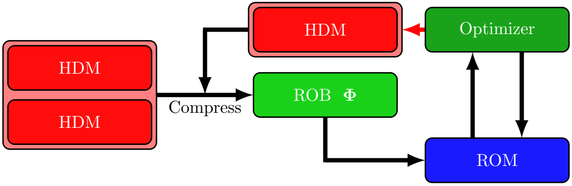


Schematic

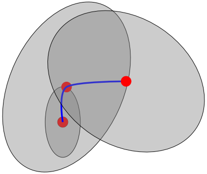


μ-space

Breakdown of Computational Effort



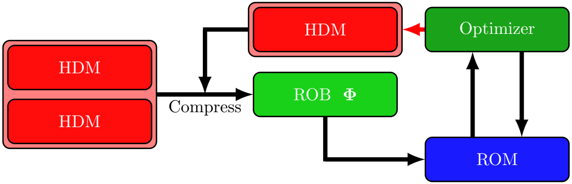
Schematic



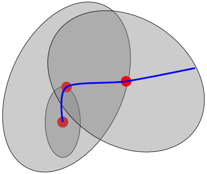
$\boldsymbol{\mu}$-space

Breakdown of Computational Effort

Trust region framework for optimization with ROMs

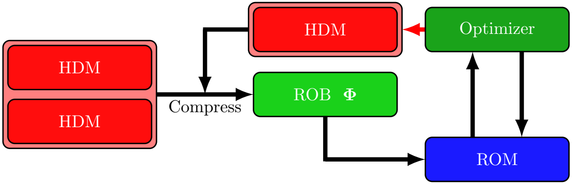


Schematic

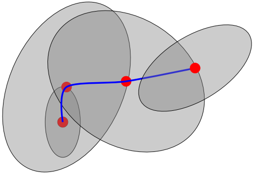


μ-space

Breakdown of Computational Effort



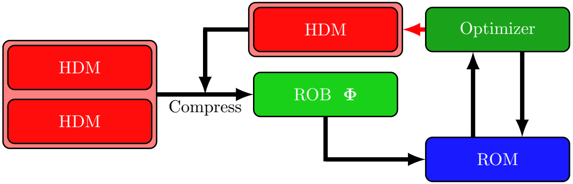
Schematic



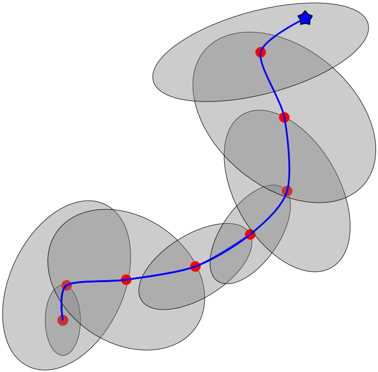
$\boldsymbol{\mu}$-space

Breakdown of Computational Effort

Trust region framework for optimization with ROMs

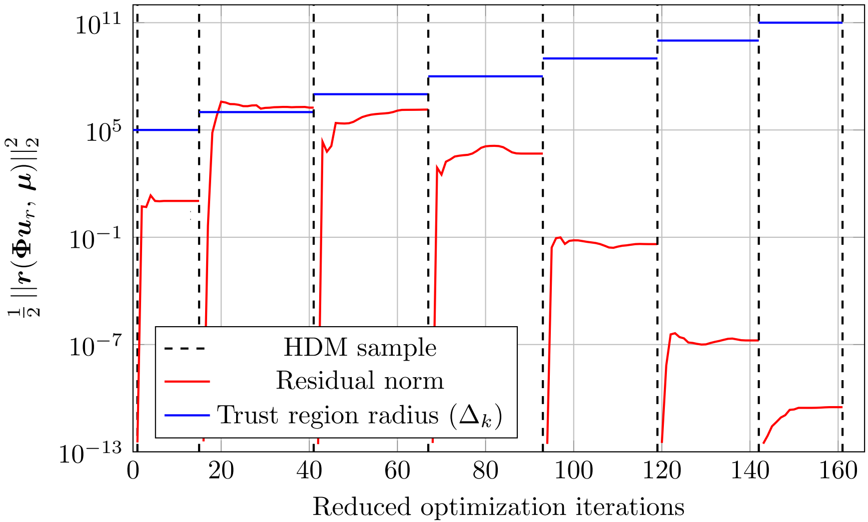


Schematic



$\boldsymbol{\mu}$-space

Breakdown of Computational Effort



10^{11}
10^{5}
10^{-1}
10^{-7}
10^{-13}
0
20
40
60
80
100
120
140
160
Reduced optimization iterations
$\frac{1}{2}||\boldsymbol{r}(\boldsymbol{\Phi}\boldsymbol{u}_r, \boldsymbol{\mu})||_2^2$
HDM sample
Residual norm
Trust region radius (Δ_k)

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 $\mathcal{I} \subset \mathbb{N}^{n_{\boldsymbol{\xi}}}$ and

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

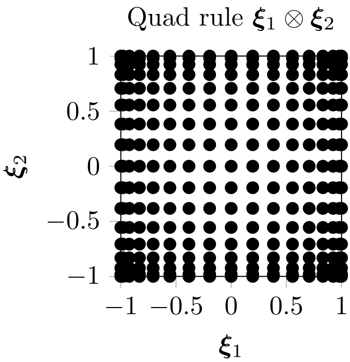
Neighbors: Let $\mathcal{I}^c = \mathbb{N}^{n_{\boldsymbol{\xi}}} \setminus \mathcal{I}$

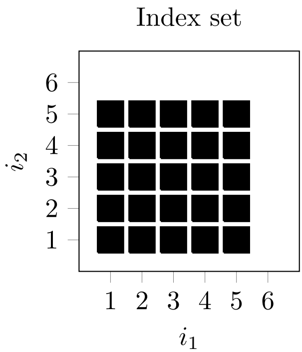
$$\mathcal{N}(\mathcal{I}) = \{\boldsymbol{i} \in \mathcal{I}^c \mid \boldsymbol{i} - \boldsymbol{e}_j \in \mathcal{I},\, j = 1,\, \ldots,\, n_{\boldsymbol{\xi}}\}$$

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

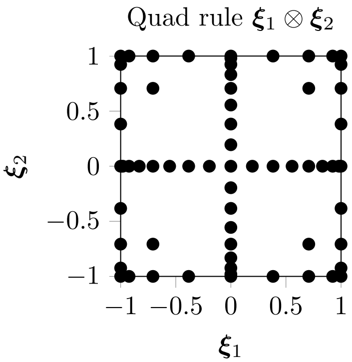
$$\mathbb{E} - \mathbb{E}_{\mathcal{I}} = \sum_{\mathbf{i}\in\mathcal{I}^c} \Delta_1^{i_1} \otimes \cdots \otimes \Delta_{n_{\boldsymbol{\xi}}}^{i_{n_{\boldsymbol{\xi}}}} \approx \sum_{\mathbf{i}\in\mathcal{N}(\mathcal{I})} \Delta_1^{i_1} \otimes \cdots \otimes \Delta_{n_{\boldsymbol{\xi}}}^{i_{n_{\boldsymbol{\xi}}}}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

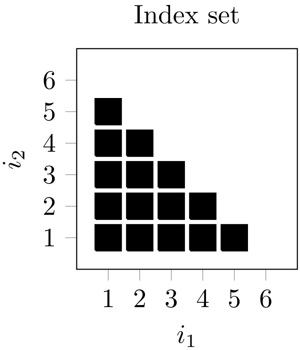
Tensor product quadrature





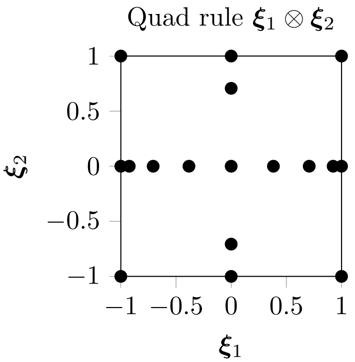
Index set ($\mathcal{I}$) – ● Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

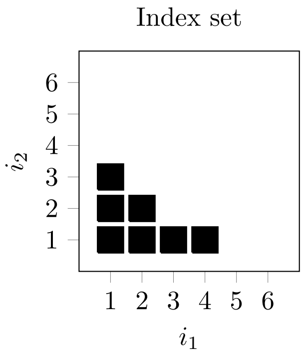




Index set $(\mathcal{I})$ – ● Neighbors $(\mathcal{N}(\mathcal{I}))$ – ●

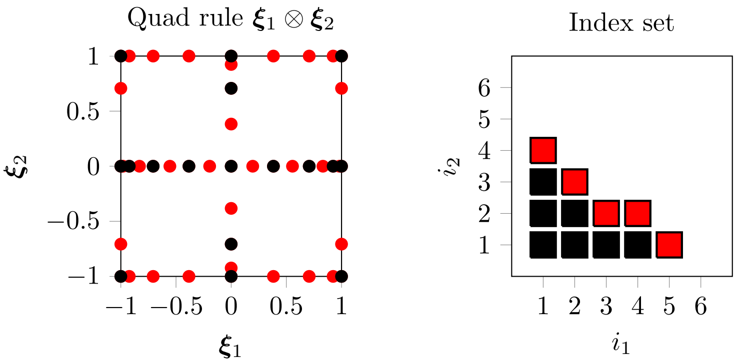
Anisotropic sparse grid quadrature





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

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

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

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

Separate total error into contributions from ROM inexactness and SG truncation

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

Derivation of gradient error indicator

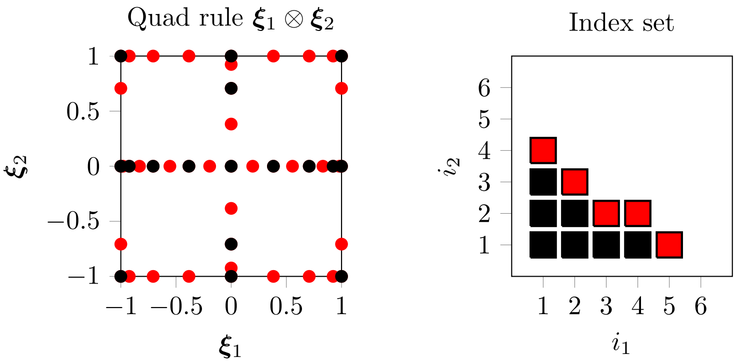
For brevity, let

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

Separate total error into contributions from ROM inexactness and SG truncation

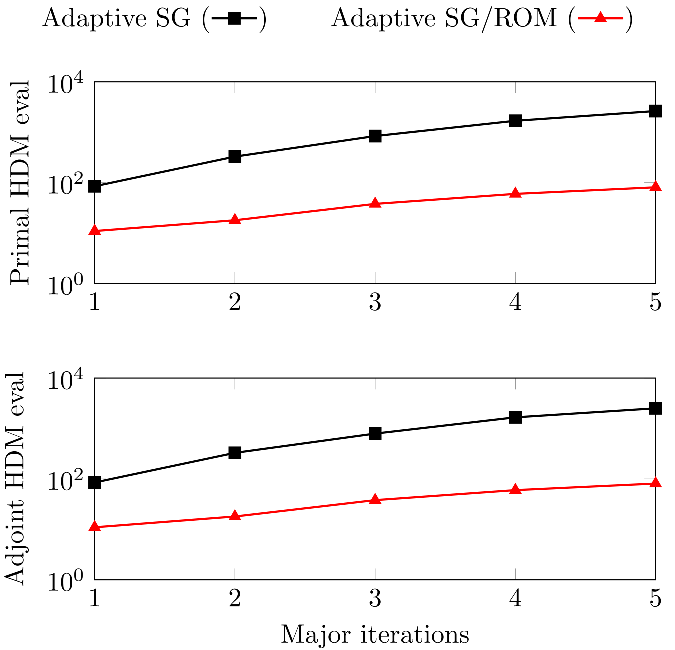
$$\begin{aligned}
||\mathbb{E}[\nabla\mathcal{J}] - \mathbb{E}_{\mathcal{I}}[\nabla\mathcal{J}_r]|| &\leq \mathbb{E}\left[||\nabla\mathcal{J} - \nabla\mathcal{J}_r||\right] + ||\mathbb{E}\left[\nabla\mathcal{J}_r\right] - \mathbb{E}_{\mathcal{I}}\left[\nabla\mathcal{J}_r\right]||\\
&\leq \zeta'\mathbb{E}\left[\alpha_1\,||\boldsymbol{r}||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

Adaptivity: Dimension-adaptive greedy method

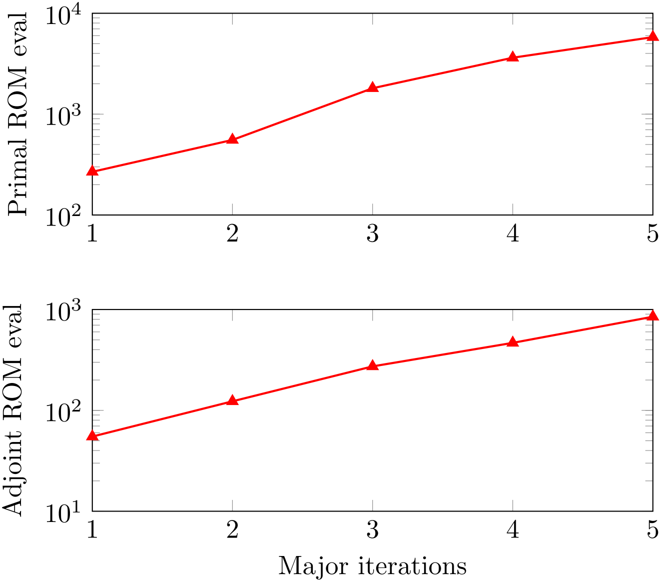


Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

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