Efficient PDE-constrained optimization under uncertainty using adaptive model reduction and sparse grids

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Aerodynamic design: maximum lift-to-drag ratio

Maximum lift-to-drag airfoil configuration

Energetically optimal flapping motions

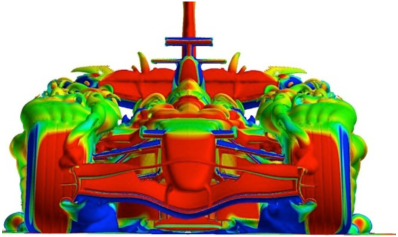
Energy = 9.4096e+00	Energy = 4.9476e+00	Energy = 4.6110e+00
Thrust = 1.7660e-01	Thrust = 2.5000e+00	Thrust = 2.5000e+00
Initial	Optimal Control	Optimal Shape/Control

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

Deterministic PDE-constrained optimization formulation

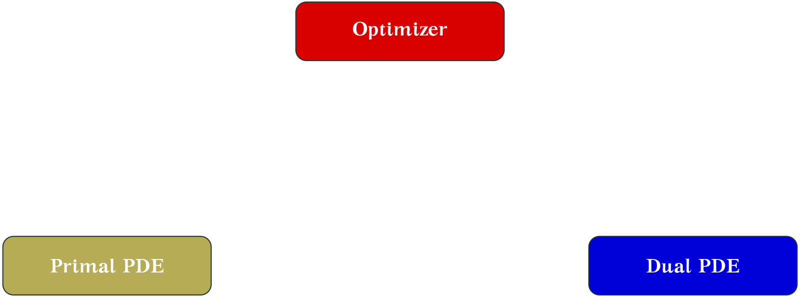
$$\begin{aligned} \underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathcal{J}(\mathbf{u}, \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{r}(\mathbf{u}; \boldsymbol{\mu}) = 0 \end{aligned}$$

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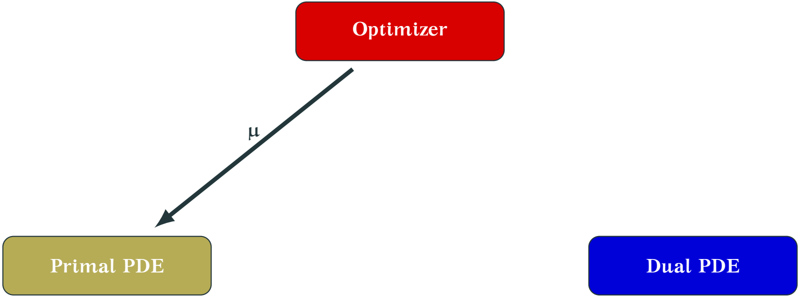

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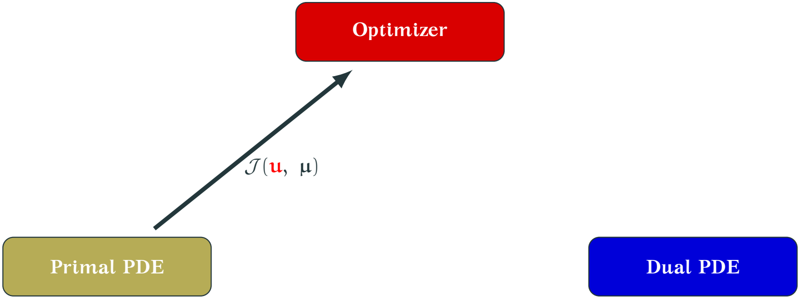

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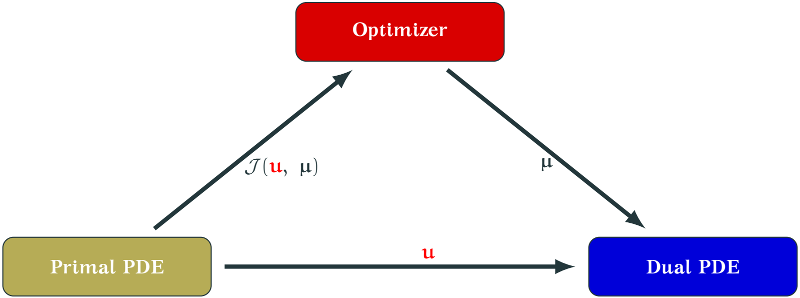

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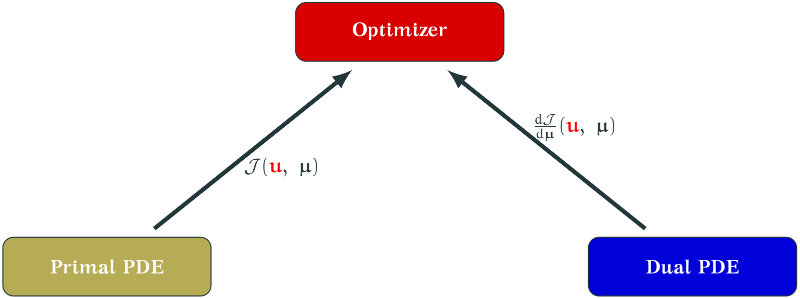
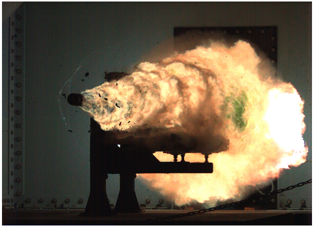


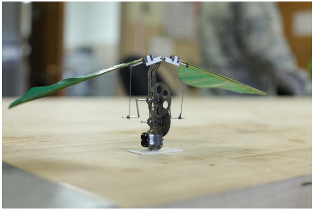
PDE optimization – a key player in next-gen problems

*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**

Stochastic PDE-constrained optimization formulation

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

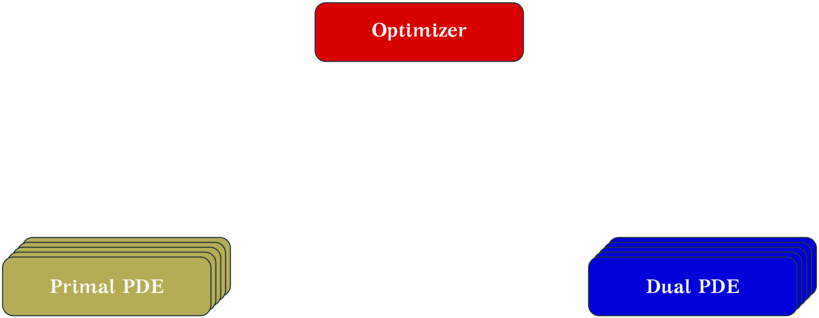
$$\text{subject to} \quad \mathbf{r}(\mathbf{u}; \boldsymbol{\mu}, \boldsymbol{\xi}) = 0 \quad \forall \boldsymbol{\xi} \in \boldsymbol{\Xi}$$

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

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

Nested approach to stochastic PDE-constrained optimization

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



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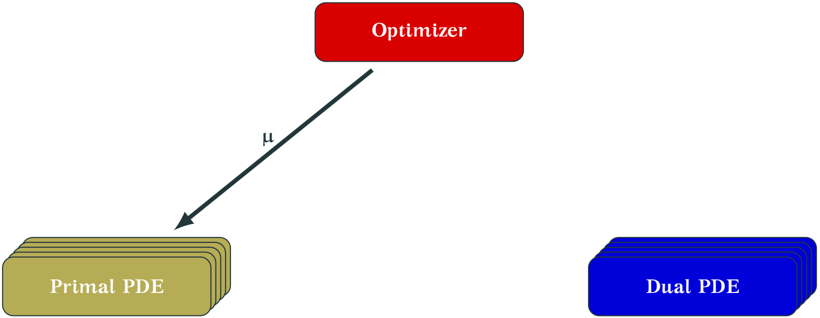

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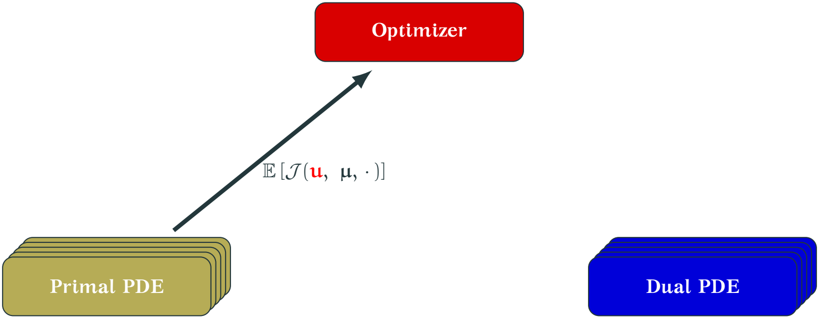

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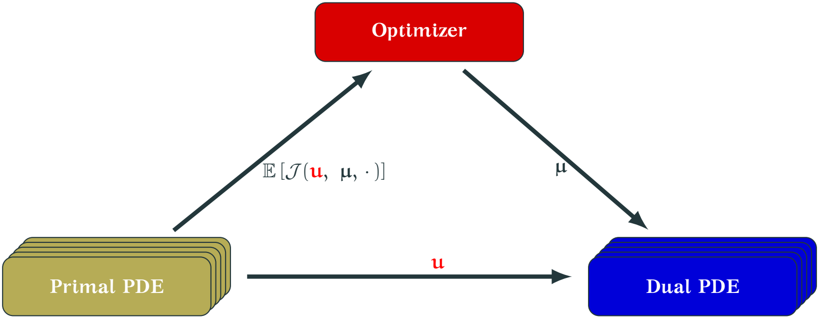

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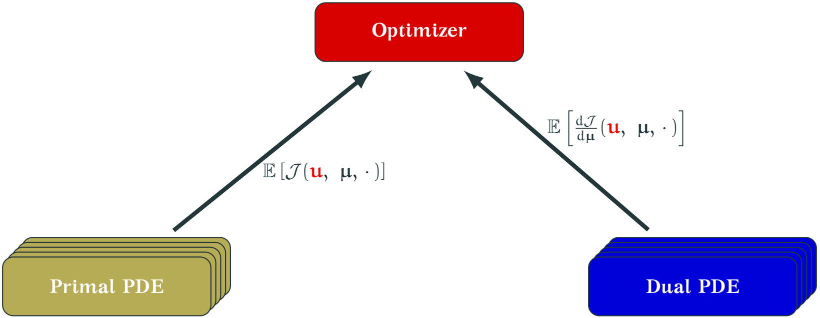

Proposed approach: managed inexactness

Replace expensive PDE with inexpensive approximation model

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

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

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

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Manage inexactness with trust region method

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

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

[1] 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

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

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

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

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

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

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

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

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

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

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

4: **Trust region update**:

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

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

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

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

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

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Trust region method with inexact gradients and objective

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

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

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

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

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

4: **Trust region update**:

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

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

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

Inexact objective evaluations with asymptotic error bounds

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

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

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

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

Trust region ingredients for global convergence

Approximation models

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

Error indicators

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

Adaptivity

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

Global convergence

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

Stochastic PDE-constrained optimization formulation

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

- $\mathbf{r} : \mathbb{R}^{n_u} \times \mathbb{R}^{n_\mu} \times \mathbb{R}^{n_\xi} \rightarrow \mathbb{R}^{n_u}$ — 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
- $\mu \in \mathbb{R}^{n_\mu}$ — (deterministic) optimization parameters
- $\xi \in \mathbb{R}^{n_\xi}$ — stochastic parameters
- $\mathbb{E}[\mathcal{F}] \equiv \int_\Xi \mathcal{F}(\xi)\rho(\xi)\, d\xi$

First source of inexactness: anisotropic sparse grids

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

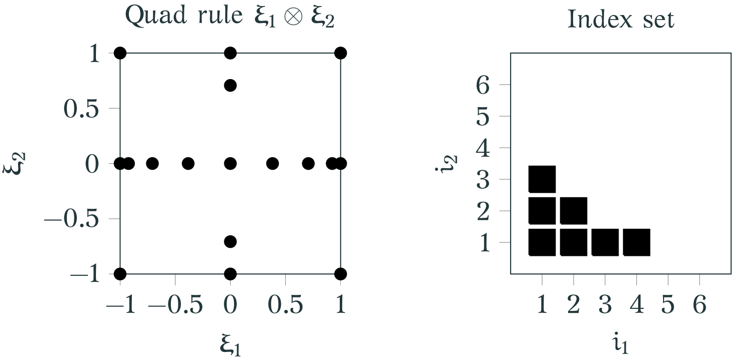
$$\begin{aligned}\underset{\mathbf{u}\in\mathbb{R}^{n_\mathbf{u}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathbb{E}[\mathcal{J}(\mathbf{u},\boldsymbol{\mu},\cdot)] \\ \text{subject to} \quad & \mathbf{r}(\mathbf{u},\boldsymbol{\mu},\boldsymbol{\xi}) = 0 \quad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

$$\Downarrow$$

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

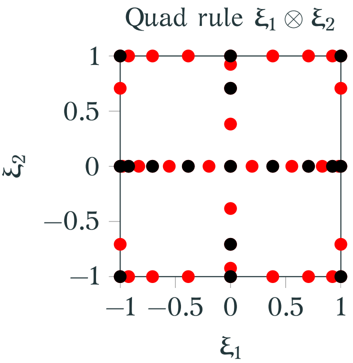
[Kouri et al., 2013, Kouri et al., 2014]

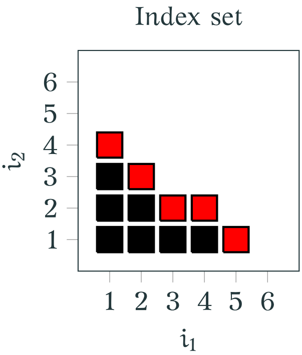
Source of inexactness: anisotropic sparse grids



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

Source of inexactness: anisotropic sparse grids





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

Second source of inexactness: reduced-order models

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

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

$$\Downarrow$$

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

$$\Downarrow$$

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

Source of inexactness: projection-based model reduction

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

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

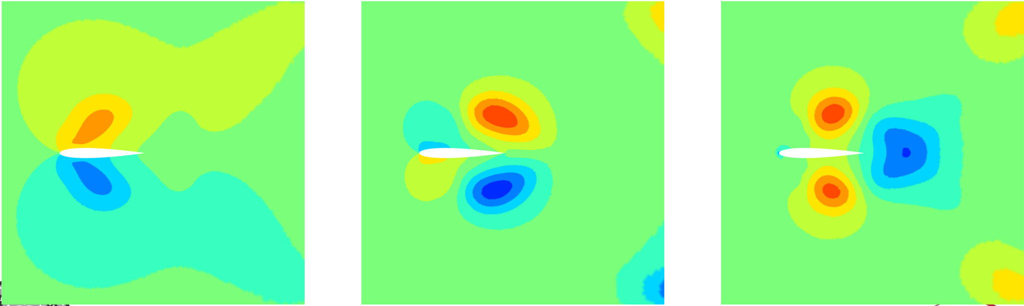
  - $\boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\phi}^1 & \cdots & \boldsymbol{\phi}^{k_u} \end{bmatrix} \in \mathbb{R}^{n_u \times k_u}$ is the reduced (trial) basis ($n_u \gg k_u$)
  - $\mathbf{u}_r \in \mathbb{R}^{k_u}$ are the reduced coordinates of $\mathbf{u}$

- Substitute into $\mathbf{r}(\mathbf{u}, \boldsymbol{\mu}) = 0$ and perform Galerkin projection

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

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

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



Trust region ingredients for global convergence

Approximation models

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

Error indicators

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

Adaptivity

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

Global convergence

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

Trust region method: ROM/SG approximation model

Approximation models built on two sources of inexactness

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

Error indicators that account for both sources of error

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

Reduced-order model errors

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

Sparse grid truncation errors

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

Final requirement for convergence: Adaptivity

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

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

the sparse grid $\mathcal{I}_k$ and reduced-order basis $\mathbf{\Phi}_k$ 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

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

Adaptivity: Dimension-adaptive greedy method

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

Refine index set: Dimension-adaptive sparse grids

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

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

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

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**

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

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

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

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

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

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**

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

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

end while

Optimal control of steady Burgers' equation

- **Optimization problem:**

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

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

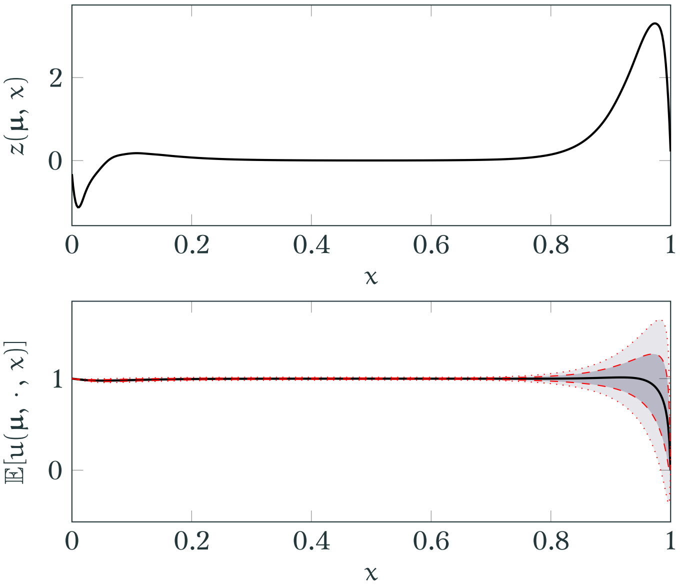
$$-\nu(\xi)\partial_{xx}u(\mu,\xi,x)+u(\mu,\xi,x)\partial_x u(\mu,\xi,x) = z(\mu,x) \quad x\in(0,1), \qquad \xi\in\Xi$$
$$u(\mu,\xi,0)=d_0(\xi) \qquad u(\mu,\xi,1)=d_1(\xi)$$

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

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

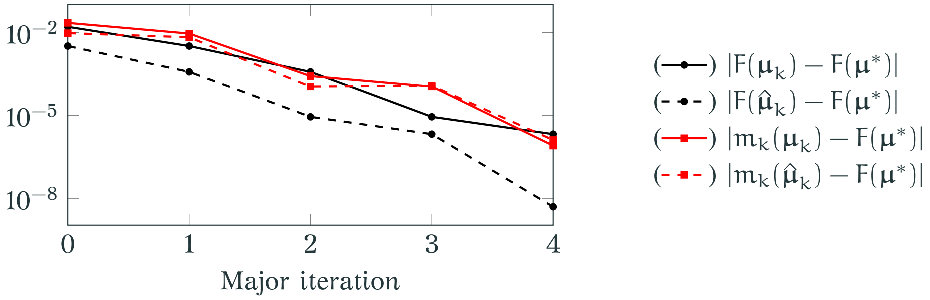
- **Parametrization:** $z(\mu, x)$ – cubic splines with 51 knots, $n_\mu = 53$

Optimal control and statistics



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

Global convergence without pointwise agreement

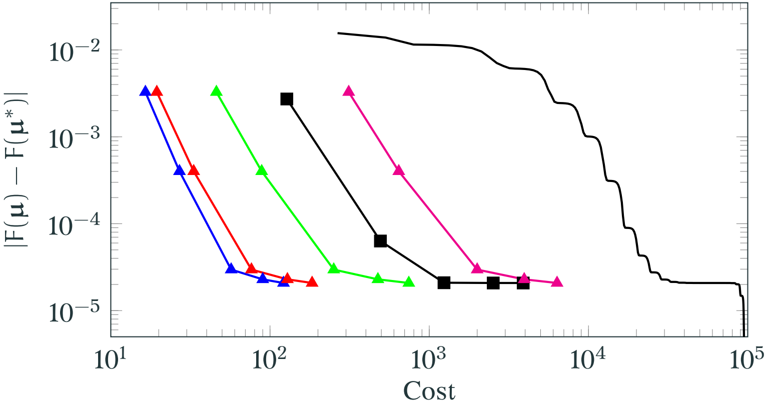


$F(\mu_k)$	$m_k(\mu_k)$	$F(\hat{\mu}_k)$	$m_k(\hat{\mu}_k)$	$\|\nabla F(\mu_k)\|$	ρ_k	Success?
6.6506e-02	7.2694e-02	5.3655e-02	5.9922e-02	2.2959e-02	1.0257e+00	1.0000e+00
5.3655e-02	5.9593e-02	5.0783e-02	5.7152e-02	2.3424e-03	9.7512e-01	1.0000e+00
5.0783e-02	5.0670e-02	5.0412e-02	5.0292e-02	1.9724e-03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

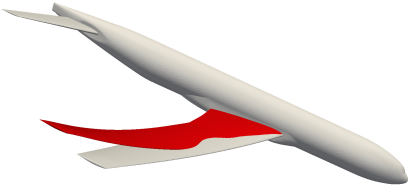
$$\text{Cost} = \text{nHdmPrim} + 0.5 \times \text{nHdmAdj} + \tau^{-1} \times (\text{nRomPrim} + 0.5 \times \text{nRomAdj})$$

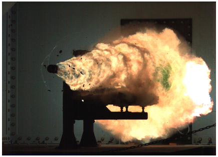


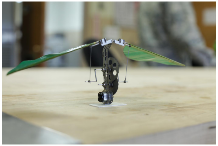
5-level isotropic SG (——), dimension-adaptive SG [Kouri et al., 2014] (—■—), and proposed ROM/SG for $\tau = 1$ (—▲—), $\tau = 10$ (—▲—), $\tau = 100$ (—▲—), $\tau = \infty$ (—▲—)

Leveraging inexactness to accelerate PDE-constrained optimization

- Framework introduced for accelerating **stochastic** PDE-constrained optimization problems
  - Adaptive *model reduction*
  - Dimension-adaptive *sparse grids*
- Inexactness **managed** with flexible **trust region** method
- **100**× speedup on (stochastic) optimal control of 1D flow

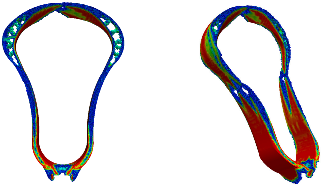


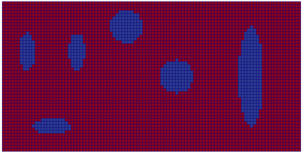


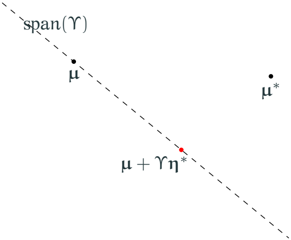


Extension to problems with many parameters

- Topology optimization[2] and inverse problems
- **Nested reduction** of state and parameter
- Multifidelity trust region method to globalize **state** reduction
- Linesearch/subspace method to globalize **parameter** reduction

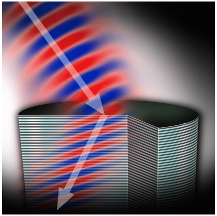
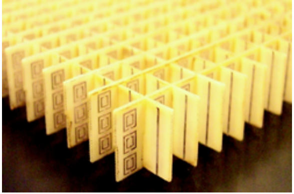




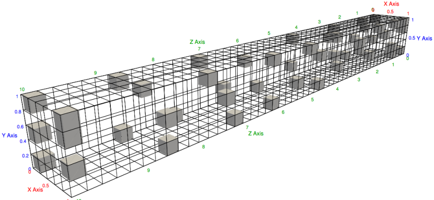


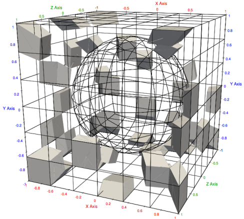
[2] Increasingly relevant due to emergence of Additive Manufacturing – *MIT Technology Review*, Top 10 Technological Breakthrough 2013

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*





Leveraging inexactness to accelerate PDE-constrained optimization

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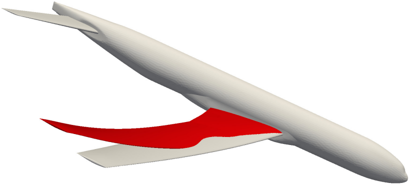

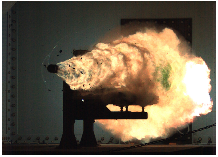

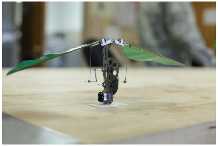

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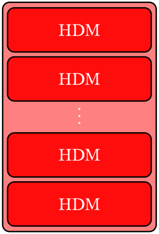
Offline-online approach to optimization with ROMs

Schematic

μ-space

Breakdown of Computational Effort

Offline-online approach to optimization with ROMs



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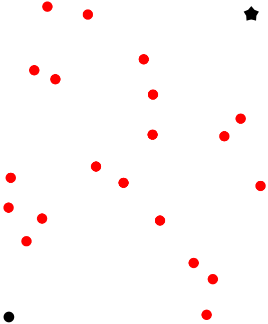

μ-space

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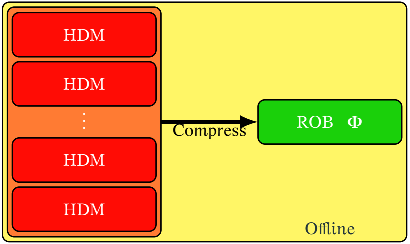

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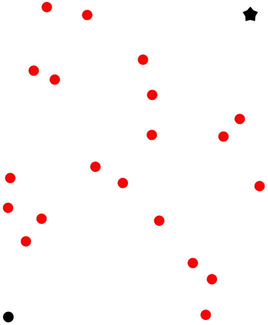

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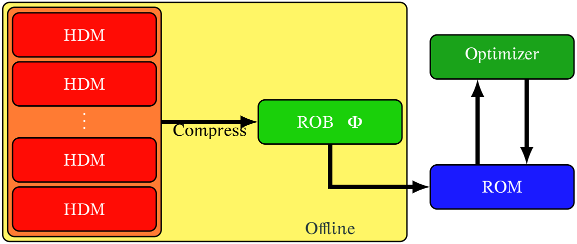

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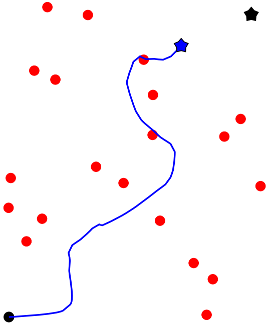

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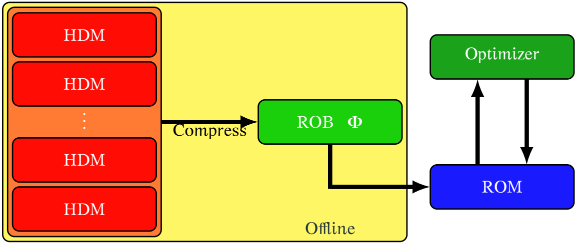

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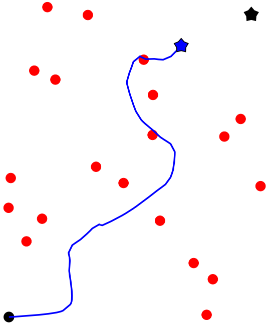


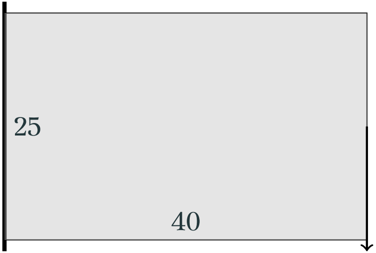
μ-space

Breakdown of Computational Effort

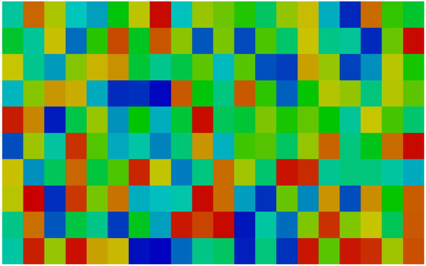
No convergence **Scales exponentially with N_μ**

Numerical demonstration: offline-online breakdown

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

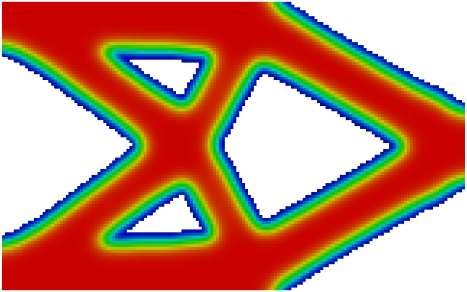


Stiffness maximization, volume constraint

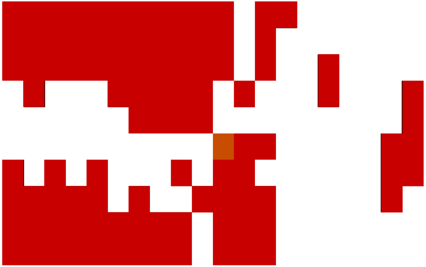


Parametrization with $n_\mu = 200$

Numerical demonstration: offline-online breakdown



Optimal Solution
(1.97×10^4 s)



ROM Solution

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

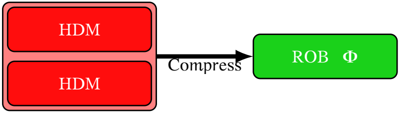
Trust region framework for optimization with ROMs

Schematic

μ-space

Breakdown of Computational Effort

Trust region framework for optimization with ROMs



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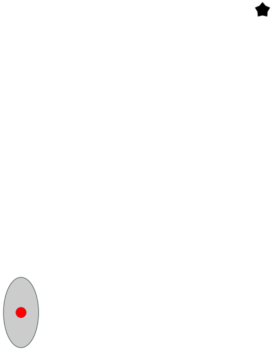

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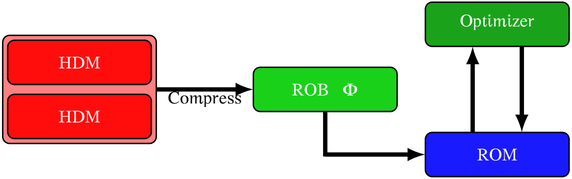

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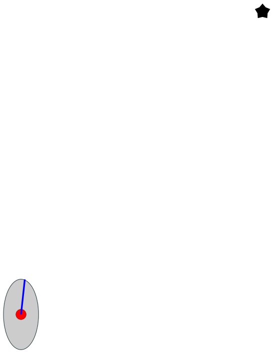

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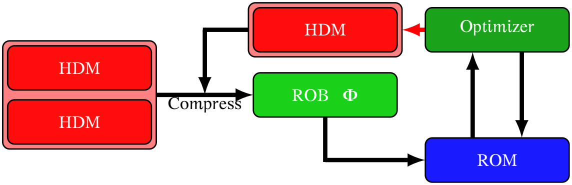

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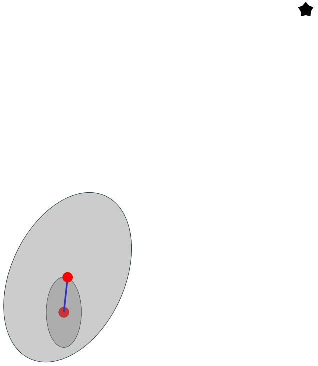

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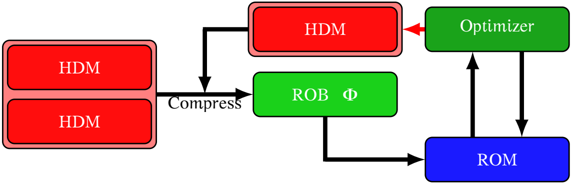
Breakdown of Computational Effort

Trust region framework for optimization with ROMs



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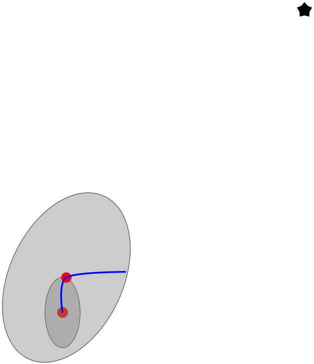

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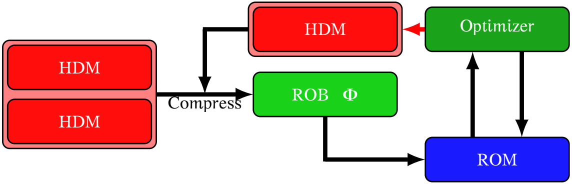

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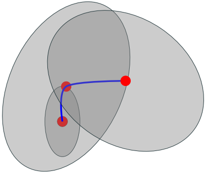

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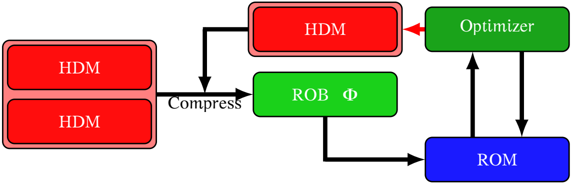

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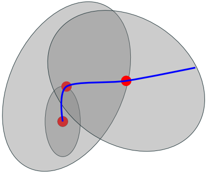

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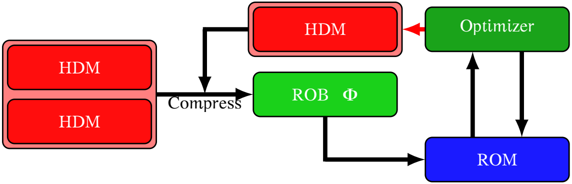

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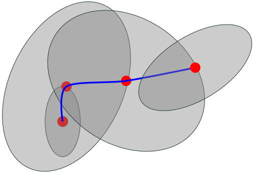

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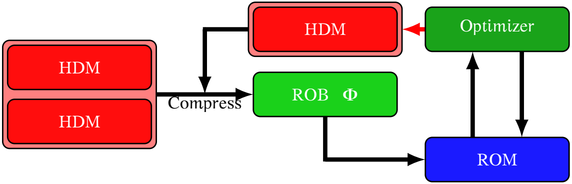

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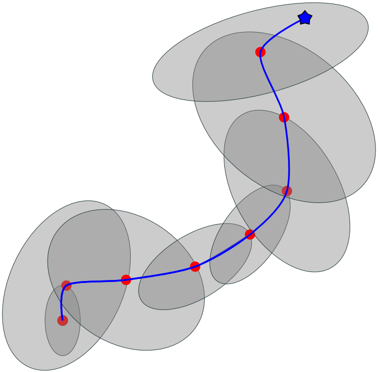


μ-space

Breakdown of Computational Effort

Source of inexactness: anisotropic sparse grids

1D Quadrature Rules: Define the difference operator

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

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

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

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

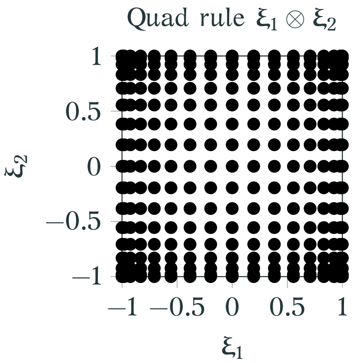
Neighbors: Let $\mathcal{I}^c = \mathbb{N}^{n_\xi} \setminus \mathcal{I}$

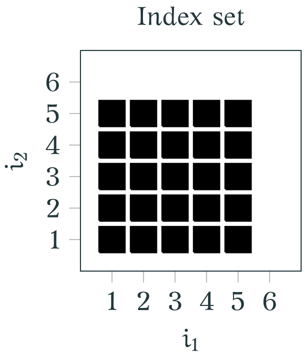
$$\mathcal{N}(\mathcal{I}) = \{\mathbf{i} \in \mathcal{I}^c \mid \mathbf{i} - \mathbf{e}_j \in \mathcal{I},\ j = 1, \ldots, n_\xi\}$$

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

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

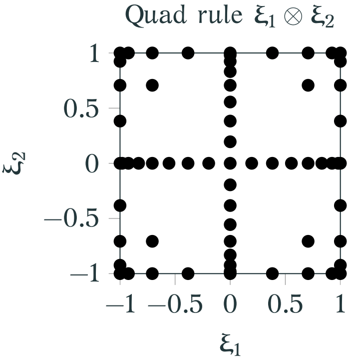
Tensor product quadrature

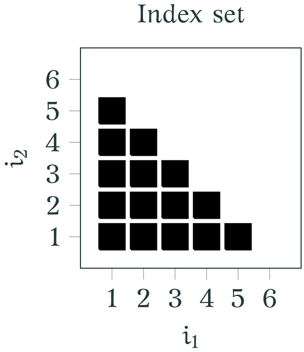




Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

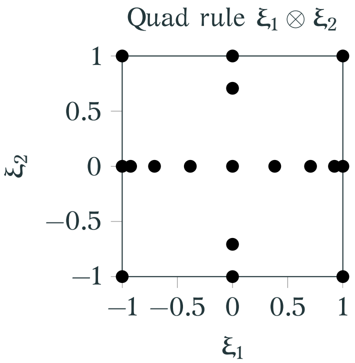
Isotropic sparse grid quadrature

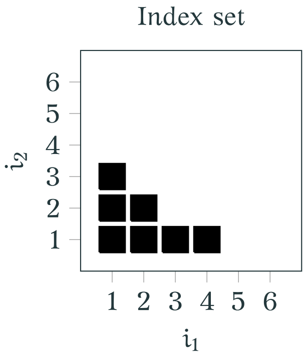




Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

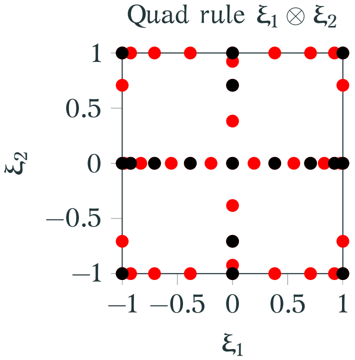
Anisotropic sparse grid quadrature

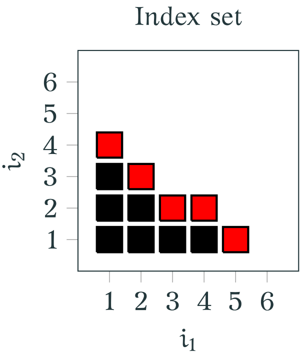




Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

Anisotropic sparse grid quadrature: neighbors





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

Derivation of gradient error indicator

For brevity, let

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

Separate total error into contributions from ROM inexactness and SG truncation

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

For brevity, let

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

Separate total error into contributions from ROM inexactness and SG truncation

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

Derivation of gradient error indicator

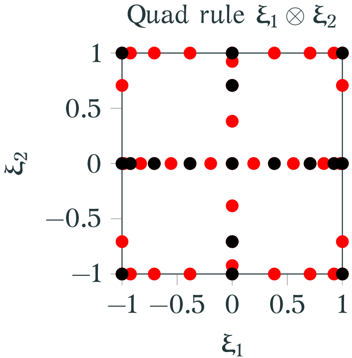
For brevity, let

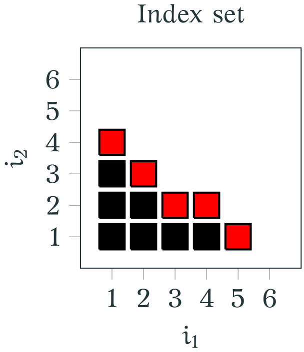
$$\begin{aligned}
\mathcal{J}(\xi) &\leftarrow \mathcal{J}(\mathbf{u}(\mu, \xi), \mu, \xi) \\
\nabla\mathcal{J}(\xi) &\leftarrow \nabla\mathcal{J}(\mathbf{u}(\mu, \xi), \mu, \xi) \\
\mathcal{J}_r(\xi) &= \mathcal{J}(\mathbf{\Phi}\mathbf{u}_r(\mu, \xi), \mu, \xi) \\
\nabla\mathcal{J}_r(\xi) &= \nabla\mathcal{J}(\mathbf{\Phi}\mathbf{u}_r(\mu,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

Separate total error into contributions from ROM inexactness and SG truncation

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

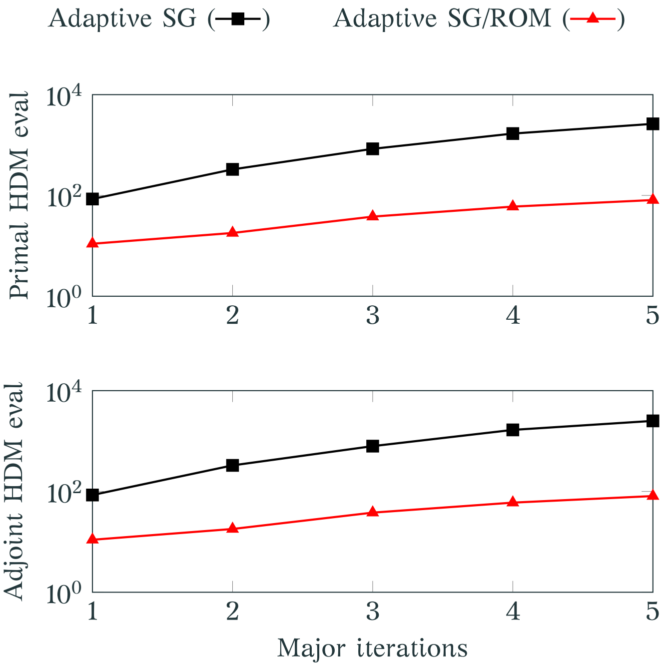
Adaptivity: Dimension-adaptive greedy method



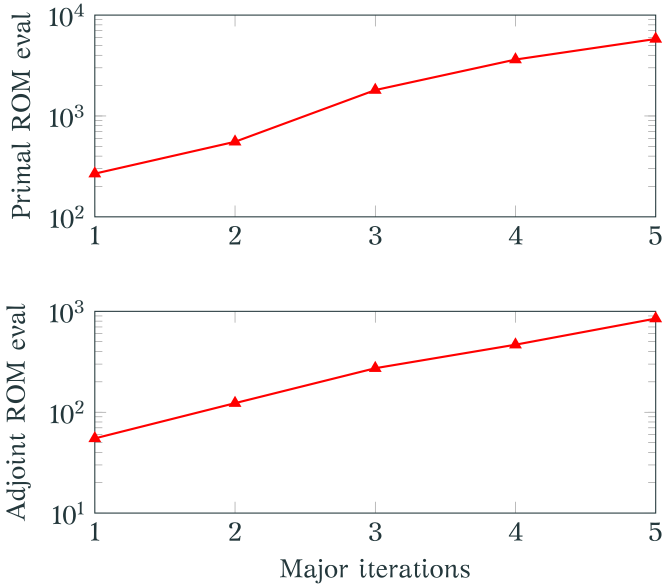


Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

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



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



Extension to time-dependent problems

- **Applications**: inverse problems, optimal flapping flight and swimming[3] 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)

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