

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

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BIRS Workshop: Data-Driven Methods for ROMs and Stochastic PDEs

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Energetically optimal flapping motions

Goal: Find energetically optimal flapping motion that achieves zero thrust

Energy = 1.4459e-01

Thrust = -1.1192e-01

Energy = 3.1378e-01

Thrust = 0.0000e+00

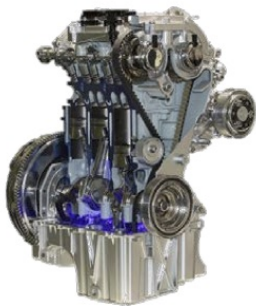


[Zahr and Persson, 2017]

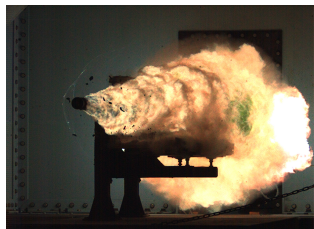


PDE optimization – a key player in next-gen problems

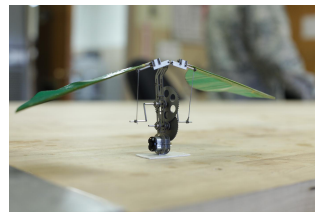
Current interest in **computational physics** reaches far beyond analysis of a single configuration of a physical system into **design** (shape and topology) and **control** in an **uncertain** setting



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

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

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

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

discretized stochastic PDE

quantity of interest

PDE state vector

(deterministic) optimization parameters

stochastic parameters



Nested approach to stochastic PDE-constrained optimization

Ensemble of primal/dual PDE solves required at **every** optimization iteration



Optimizer

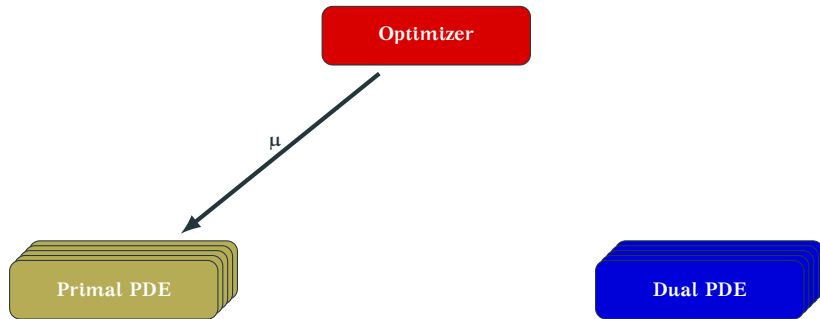
Primal PDE

Dual PDE



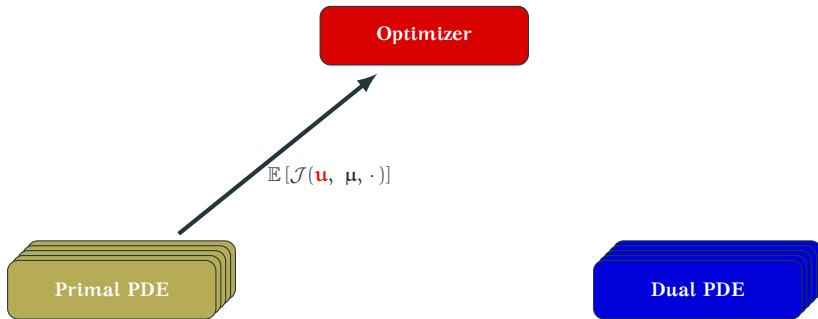
Nested approach to stochastic PDE-constrained optimization

Ensemble of primal/dual PDE solves required at **every** optimization iteration



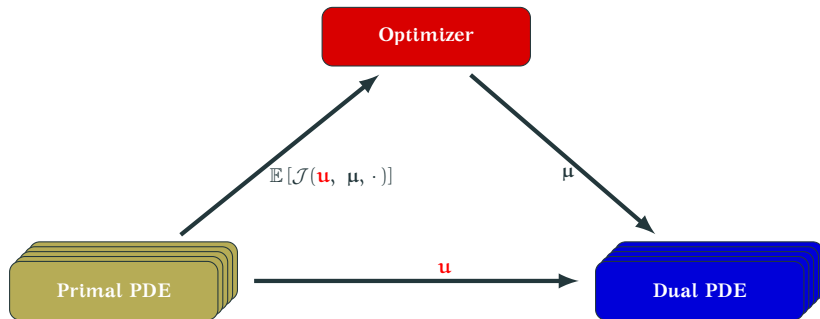
Nested approach to stochastic PDE-constrained optimization

Ensemble of primal/dual PDE solves required at **every** optimization iteration



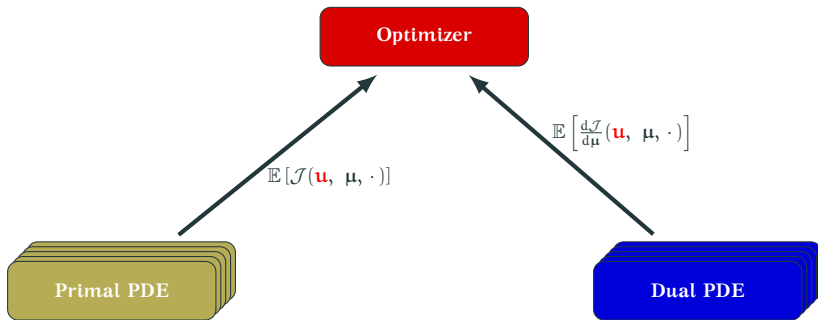
Nested approach to stochastic PDE-constrained optimization

Ensemble of primal/dual PDE solves required at **every** optimization iteration



Nested approach to stochastic PDE-constrained optimization

Ensemble of primal/dual PDE solves required at **every** optimization iteration



Replace expensive PDE with inexpensive approximation model

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

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

Proposed approach: managed inexactness

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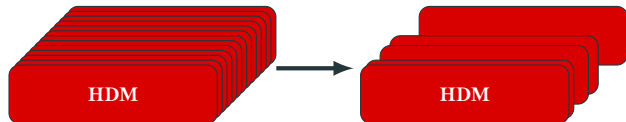


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Manage inexactness with trust region method

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

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

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

Trust region framework for optimization with ROMs



Schematic



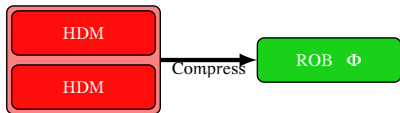
μ -space



Breakdown of Computational Effort



Trust region framework for optimization with ROMs



Schematic



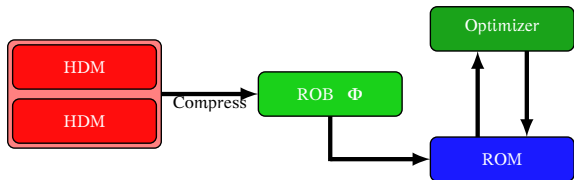
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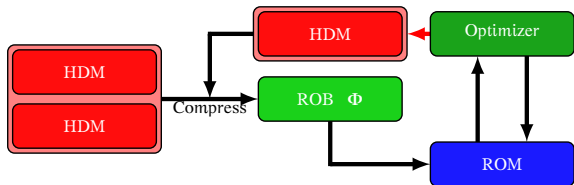
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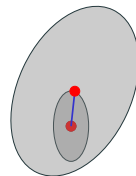
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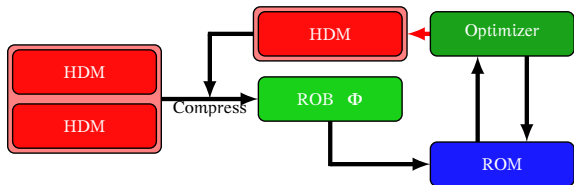
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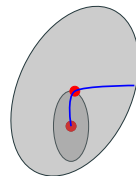
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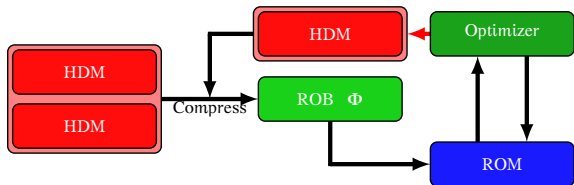
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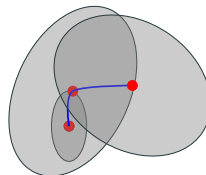
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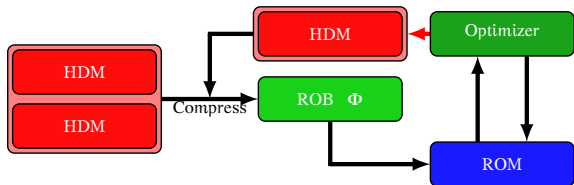
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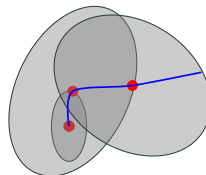
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Schematic



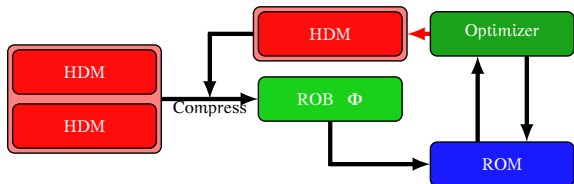
μ -space



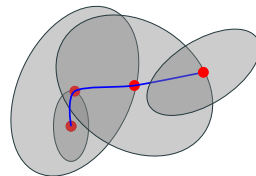
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Trust region framework for optimization with ROMs



Schematic



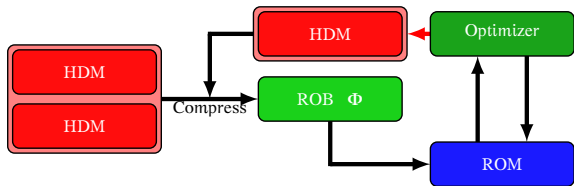
μ -space



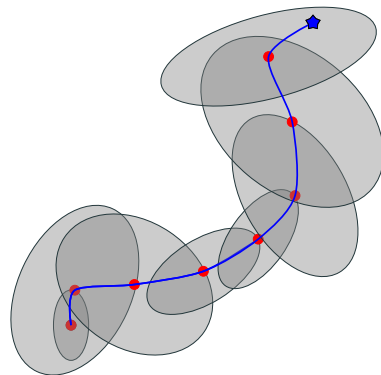
Breakdown of Computational Effort



Trust region framework for optimization with ROMs



Schematic



μ -space



Breakdown of Computational Effort



- **Stochastic collocation**

- Dimension-adaptive sparse grids – globalized with trust-region method [Kouri et al., 2013, Kouri et al., 2014]
- Generalized polynomial chaos – sequential quadratic programming [Tiesler et al., 2012]
- + *Orders of magnitude improvement over isotropic sparse grids*
- *Still requires many PDE solves for even moderate dimensional problems*

- **Model order reduction**

- Goal-oriented, dimension-adaptive, weighted greedy algorithm for training stochastic reduced-order model [Chen and Quarteroni, 2015]
- Extension to optimal control [Chen and Quarteroni, 2014]
- + *Reduction in number of PDE solves at cost of large number of ROM solves*
- *Restriction to offline-online framework may lead to unnecessary PDE solves and large reduced bases*





Schematic



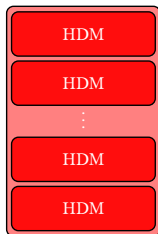
μ -space



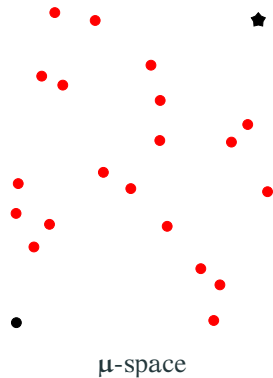
Breakdown of Computational Effort



Offline-online approach to optimization with ROMs



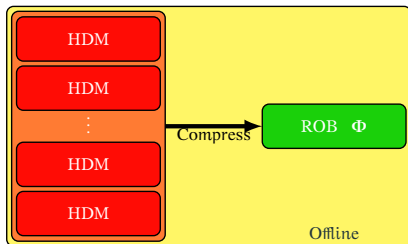
Schematic



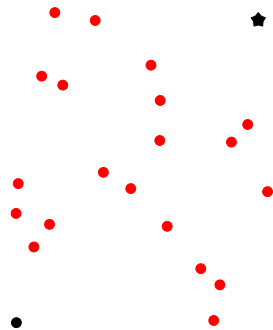
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Offline-online approach to optimization with ROMs



Schematic



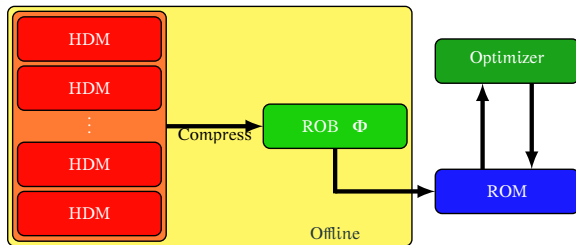
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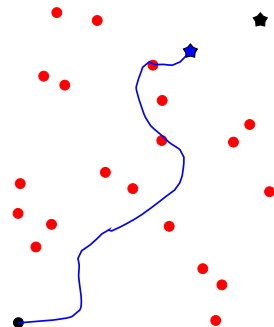
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Schematic



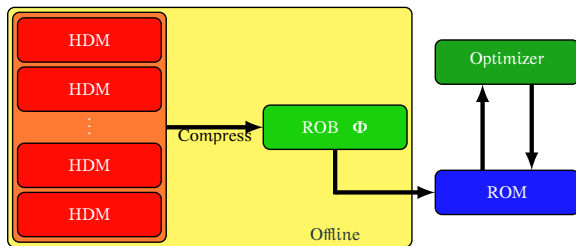
μ -space



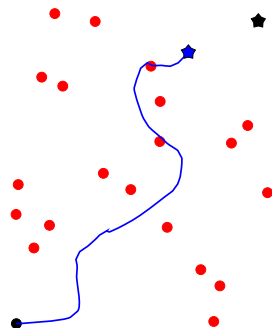
Breakdown of Computational Effort



Offline-online approach to optimization with ROMs



Schematic



μ -space



Breakdown of Computational Effort

No general convergence

Scales exponentially with n_μ



Proposed approach: managed inexactness

Replace expensive PDE with inexpensive approximation model

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

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

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- **Error indicators**² to account for *all* sources of inexactness
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²Must be *computable* and apply to general, nonlinear PDEs

First source of inexactness: anisotropic sparse grids

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

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

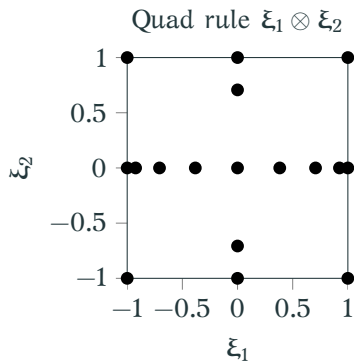
\Downarrow

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

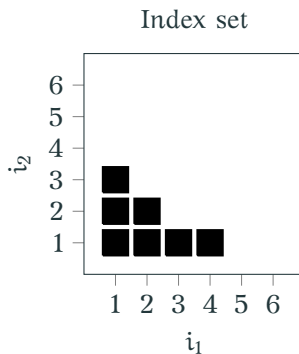
[Kouri et al., 2013, Kouri et al., 2014]



Source of inexactness: anisotropic sparse grids



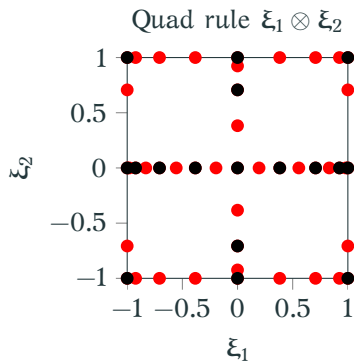
Index set (\mathcal{I}) - ●



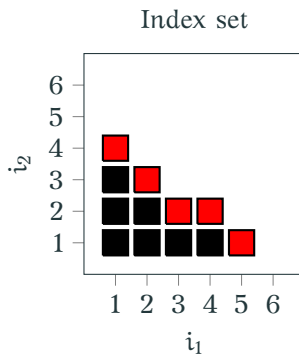
Neighbors ($\mathcal{N}(\mathcal{I})$) - ●



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

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



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



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



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

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

- $\Phi = \begin{bmatrix} \phi^1 & \dots & \phi^{k_u} \end{bmatrix} \in \mathbb{R}^{n_u \times k_u}$ 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

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



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

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- **Error indicators**³ to account for *all* sources of inexactness
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³Must be *computable* and apply to general, nonlinear PDEs

Trust region ingredients for global convergence

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

Approximation models

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

Error indicators

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

Adaptivity

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



Trust region method with inexact gradients and objective

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

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

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** $\Delta_{k+1} \in (0, \gamma \|\hat{\boldsymbol{\mu}}_k - \boldsymbol{\mu}_k\|)$ **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**



Trust region ingredients for global convergence

Approximation models

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

Error indicators

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

$$|F(\boldsymbol{\mu}_k) - F(\boldsymbol{\mu}) + \psi_k(\boldsymbol{\mu}) - \psi_k(\boldsymbol{\mu}_k)| \leq \sigma \theta_k(\boldsymbol{\mu}) \quad \sigma > 0$$

Adaptivity

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

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

Global convergence

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



Trust region method: ROM/SG approximation model

Approximation models built on two sources of inexactness

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

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

Error indicators that account for both sources of error

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

$$\theta_k(\boldsymbol{\mu}) = \beta_1 (\mathcal{E}_1(\boldsymbol{\mu}; \mathcal{I}'_k, \Phi'_k) + \mathcal{E}_1(\boldsymbol{\mu}_k; \mathcal{I}'_k, \Phi'_k)) + \beta_2 (\mathcal{E}_3(\boldsymbol{\mu}; \mathcal{I}'_k, \Phi'_k) + \mathcal{E}_3(\boldsymbol{\mu}_k; \mathcal{I}'_k, \Phi'_k))$$

Reduced-order model errors

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

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

Sparse grid truncation errors

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

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



Final requirement for convergence: Adaptivity

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

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

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

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

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

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

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

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

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



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

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



Adaptivity: Dimension-adaptive greedy method

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

Refine index set: Dimension-adaptive sparse grids

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

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

$$\Phi_k \leftarrow \left[\Phi_k \quad \mathbf{u}(\mu_k, \xi^*) \quad \lambda(\mu_k, \xi^*) \right]$$
$$\xi^* = \arg \max_{\xi \in \Xi_{j^*}} \rho(\xi) \|\mathbf{r}(\Phi_k \mathbf{u}_r(\mu_k, \xi), \mu_k, \xi)\|$$

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

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

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

$$\Phi_k \leftarrow \begin{bmatrix} \Phi_k & \mathbf{u}(\mu_k, \xi^*) & \lambda(\mu_k, \xi^*) \end{bmatrix}$$
$$\xi^* = \arg \max_{\xi \in \Xi_{\mathbf{j}^*}} \rho(\xi) \|\mathbf{r}(\Phi_k \mathbf{u}_r(\mu_k, \xi), \mu_k, \xi)\|$$

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

$$\Phi_k \leftarrow \begin{bmatrix} \Phi_k & \mathbf{u}(\mu_k, \xi^*) & \lambda(\mu_k, \xi^*) \end{bmatrix}$$
$$\xi^* = \arg \max_{\xi \in \Xi_{\mathbf{j}^*}} \rho(\xi) \|\mathbf{r}^\lambda(\Phi_k \mathbf{u}_r(\mu_k, \xi), \Phi_k \lambda_r(\mu_k, \xi), \mu_k, \xi)\|$$

end while



- **Optimization problem:**

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

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

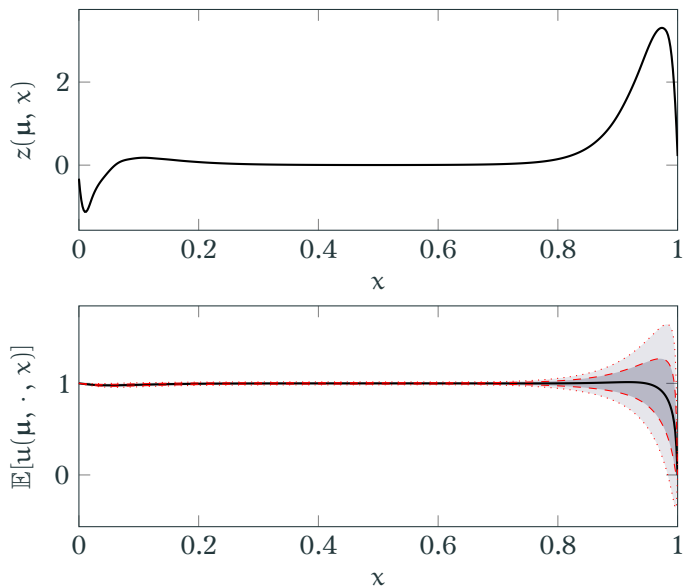
$$\begin{aligned} -\nu(\xi) \partial_{xx} u(\mu, \xi, x) + u(\mu, \xi, x) \partial_x u(\mu, \xi, x) &= z(\mu, x) \quad x \in (0, 1), \quad \xi \in \Xi \\ u(\mu, \xi, 0) &= d_0(\xi) \quad u(\mu, \xi, 1) = d_1(\xi) \end{aligned}$$

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

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

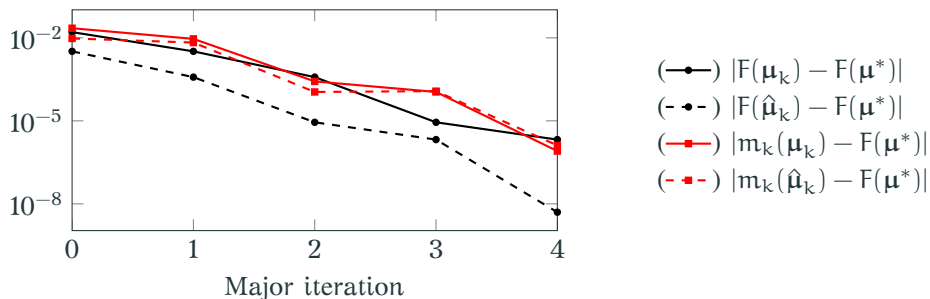
- **Parametrization:** $z(\mu, x)$ – cubic splines with 51 knots, $n_\mu = 53$





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

Global convergence without pointwise agreement

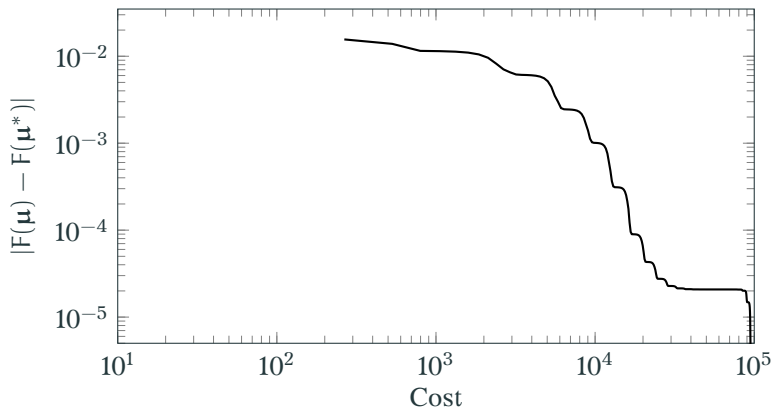


$F(\mu_k)$	$m_k(\mu_k)$	$F(\hat{\mu}_k)$	$m_k(\hat{\mu}_k)$	$\ \nabla F(\mu_k)\ $	ρ_k	Success?
6.6506e-02	7.2694e-02	5.3655e-02	5.9922e-02	2.2959e-02	1.0257e+00	1.0000e+00
5.3655e-02	5.9593e-02	5.0783e-02	5.7152e-02	2.3424e-03	9.7512e-01	1.0000e+00
5.0783e-02	5.0670e-02	5.0412e-02	5.0292e-02	1.9724e-03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

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

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

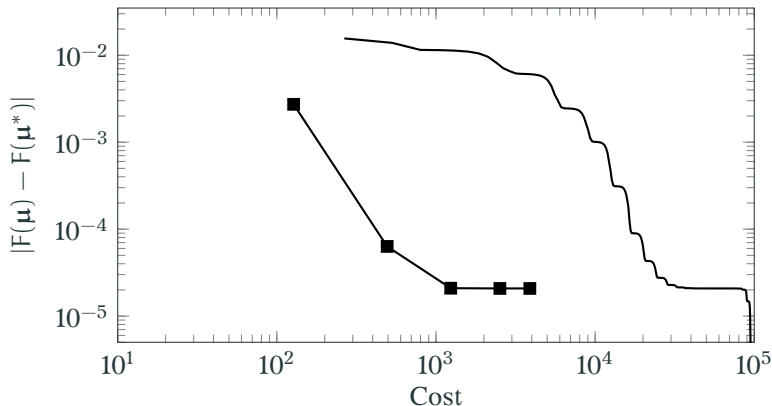
$$\text{Cost} = n_{\text{HdmPrim}} + 0.5 \times n_{\text{HdmAdj}} + \tau^{-1} \times (n_{\text{RomPrim}} + 0.5 \times n_{\text{RomAdj}})$$



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

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

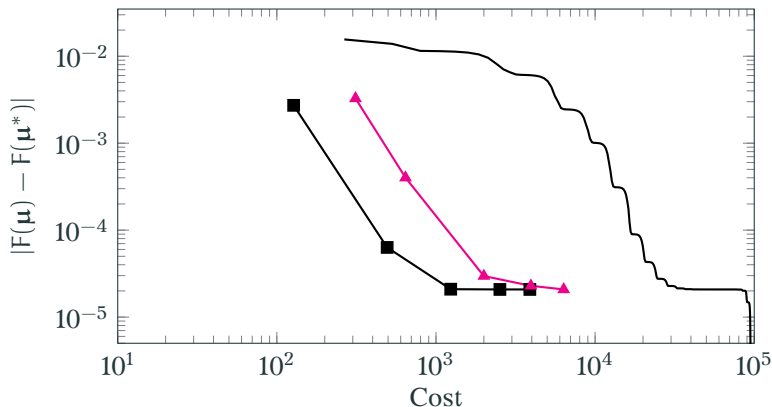
$$\text{Cost} = n_{\text{HdmPrim}} + 0.5 \times n_{\text{HdmAdj}} + \tau^{-1} \times (n_{\text{RomPrim}} + 0.5 \times n_{\text{RomAdj}})$$



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

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

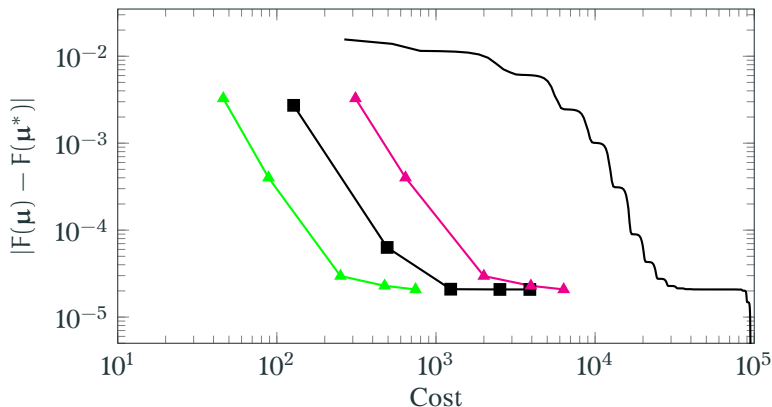
$$\text{Cost} = n_{\text{HdmPrim}} + 0.5 \times n_{\text{HdmAdj}} + \tau^{-1} \times (n_{\text{RomPrim}} + 0.5 \times n_{\text{RomAdj}})$$



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

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

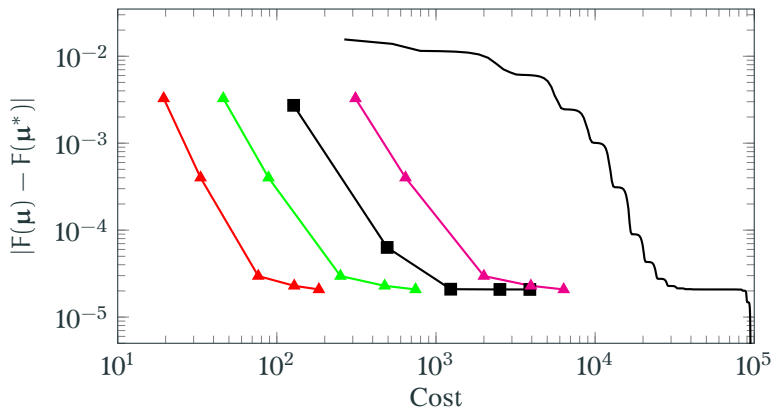
$$\text{Cost} = n_{\text{HdmPrim}} + 0.5 \times n_{\text{HdmAdj}} + \tau^{-1} \times (n_{\text{RomPrim}} + 0.5 \times n_{\text{RomAdj}})$$



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

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

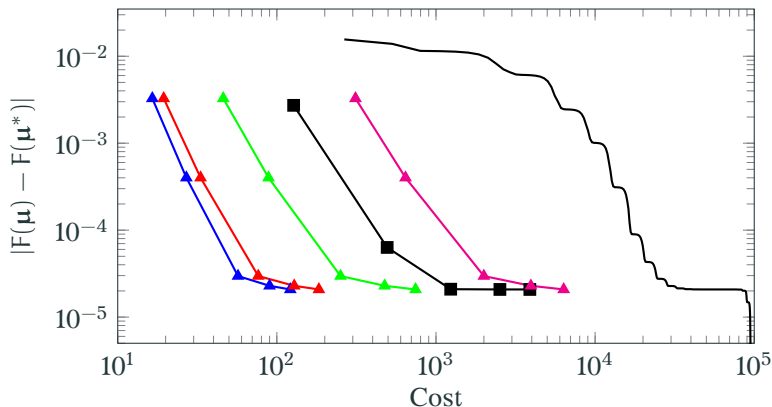
$$\text{Cost} = n_{\text{HdmPrim}} + 0.5 \times n_{\text{HdmAdj}} + \tau^{-1} \times (n_{\text{RomPrim}} + 0.5 \times n_{\text{RomAdj}})$$



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

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

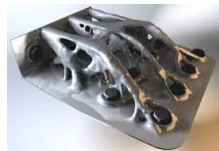
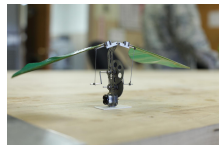
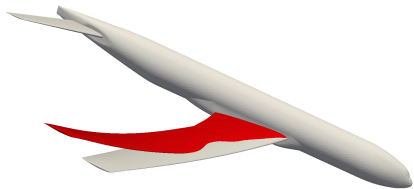
$$\text{Cost} = n_{\text{HdmPrim}} + 0.5 \times n_{\text{HdmAdj}} + \tau^{-1} \times (n_{\text{RomPrim}} + 0.5 \times n_{\text{RomAdj}})$$






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



-  Chen, P. and Quarteroni, A. (2014).
Weighted reduced basis method for stochastic optimal control problems with elliptic PDE constraint.
Siam/Asa Journal on Uncertainty Quantification, 2(1):364–396.
-  Chen, P. and Quarteroni, A. (2015).
A new algorithm for high-dimensional uncertainty quantification based on dimension-adaptive sparse grid approximation and reduced basis methods.
Journal of Computational Physics, 298:176–193.
-  Kouri, D. P., Heinkenschloss, M., Ridzal, D., and van Bloemen Waanders, B. G. (2013).
A trust-region algorithm with adaptive stochastic collocation for pde optimization under uncertainty.
SIAM Journal on Scientific Computing, 35(4):A1847–A1879.



-  Kouri, D. P., Heinkenschloss, M., Ridzal, D., and van Bloemen Waanders, B. G. (2014).

Inexact objective function evaluations in a trust-region algorithm for PDE-constrained optimization under uncertainty.

SIAM Journal on Scientific Computing, 36(6):A3011–A3029.

-  Tiesler, H., Kirby, R. M., Xiu, D., and Preusser, T. (2012).

Stochastic collocation for optimal control problems with stochastic PDE constraints.

SIAM Journal on Control and Optimization, 50(5):2659–2682.

-  Zahr, M. J. and Persson, P.-O. (2017).

Energetically optimal flapping wing motions via adjoint-based optimization and high-order discretizations.

In Frontiers in PDE-Constrained Optimization. Springer.

