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

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2017 West Coast ROM Workshop

Lawrence Berkeley National Laboratory

November 17, 2017

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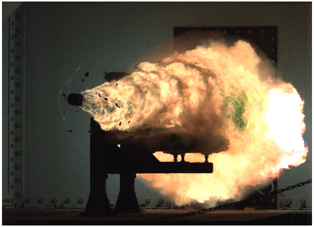
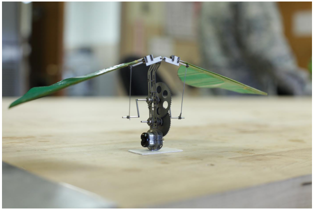
PDE optimization – a key player in next-gen problems

*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**

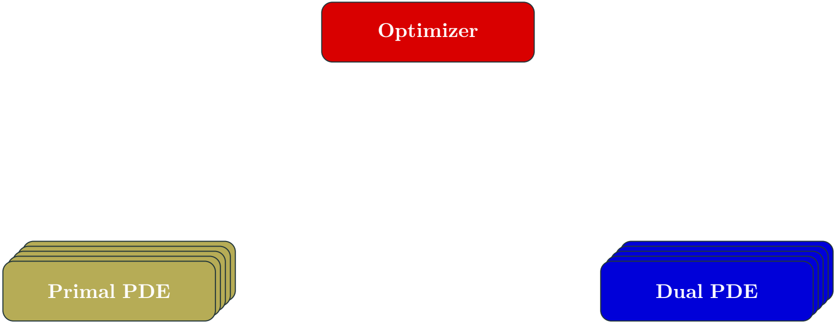
Stochastic PDE-constrained optimization formulation

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

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

Nested approach to stochastic PDE-constrained optimization

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



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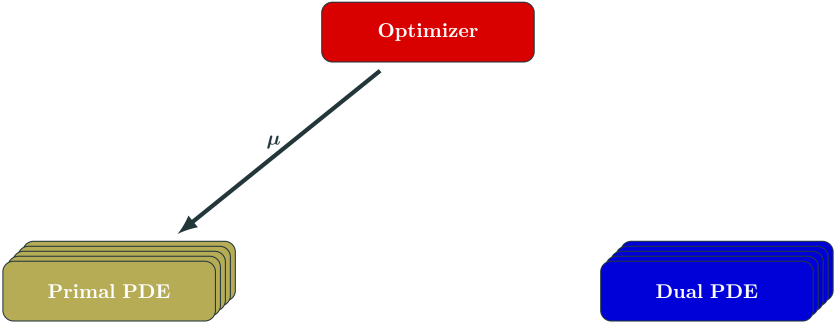

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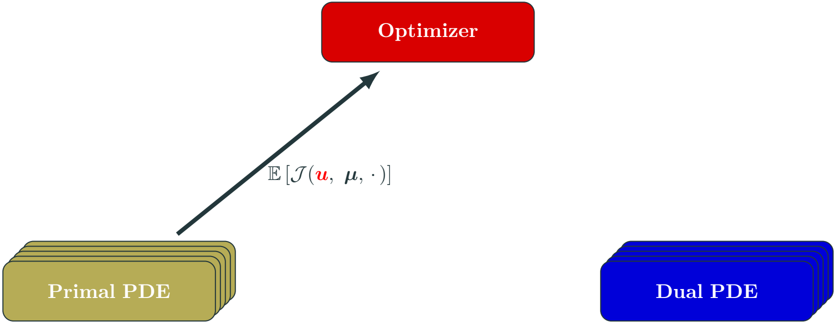

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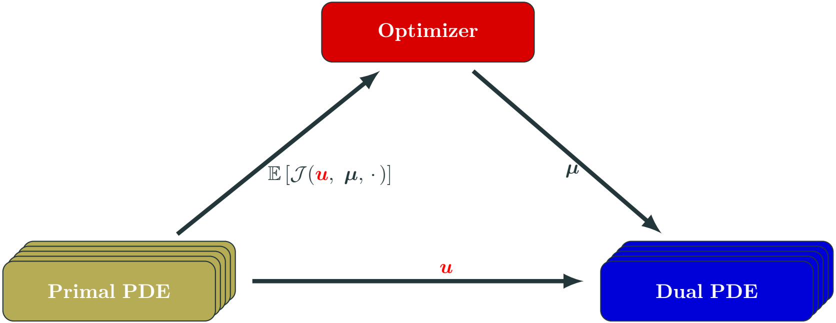

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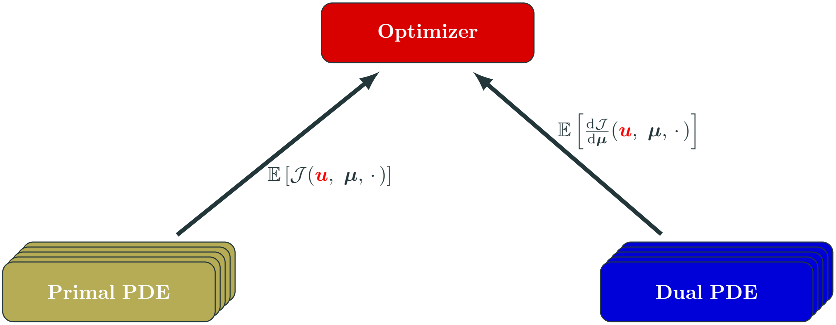

Proposed approach: managed inexactness

Replace expensive PDE with inexpensive approximation model

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

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

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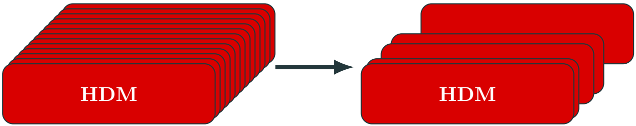

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Manage inexactness with trust region method

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

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

[1] Must 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

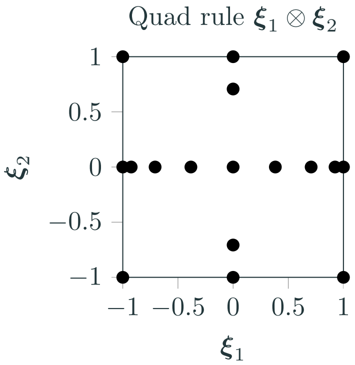
$$\begin{aligned} \underset{\boldsymbol{u}\in\mathbb{R}^{n_{\boldsymbol{u}}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathbb{E}[\mathcal{J}(\boldsymbol{u},\, \boldsymbol{\mu},\, \cdot\,)] \\ \text{subject to} \quad & \boldsymbol{r}(\boldsymbol{u},\, \boldsymbol{\mu},\,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

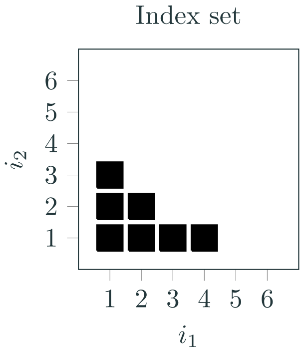
$$\Downarrow$$

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

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

Source of inexactness: anisotropic sparse grids





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

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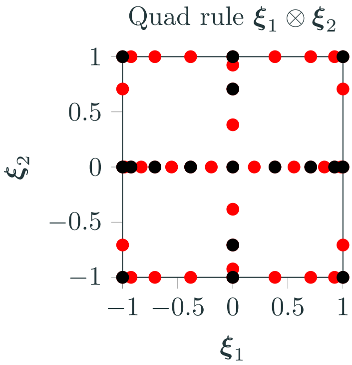

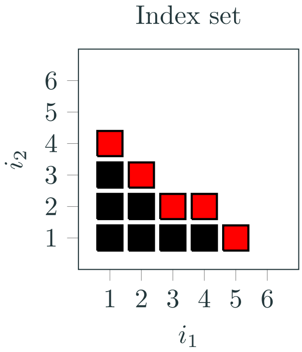

Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

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

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

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

$$\Downarrow$$

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

Source of inexactness: projection-based model reduction

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

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

  - $\boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\phi}^1 & \cdots & \boldsymbol{\phi}^{k_{\boldsymbol{u}}} \end{bmatrix} \in \mathbb{R}^{n_{\boldsymbol{u}} \times k_{\boldsymbol{u}}}$ 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 perform Galerkin projection

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

Trust region ingredients, global convergence $\left(\liminf_{k\to\infty} ||\nabla F(\boldsymbol{\mu}_k)|| = 0\right)$

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

Approximation models

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

Error indicators

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

Adaptivity

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

Trust region method: ROM/SG approximation model

Approximation models built on two sources of inexactness

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

Error indicators that account for both sources of error

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

Reduced-order model errors

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

Sparse grid truncation errors

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

Adaptivity: Dimension-adaptive greedy method

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

Refine index set: Dimension-adaptive sparse grids

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

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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

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

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end while

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

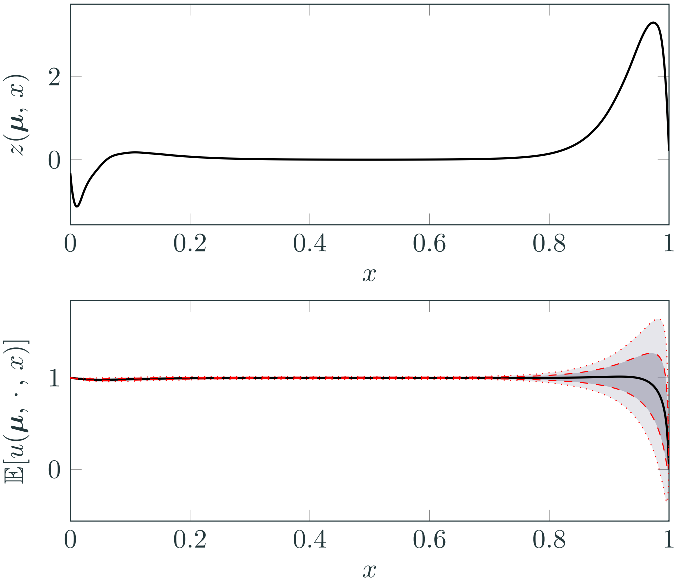
$$-\nu(\boldsymbol{\xi})\partial_{xx}u(\boldsymbol{\mu}, \boldsymbol{\xi}, x) + u(\boldsymbol{\mu}, \boldsymbol{\xi}, x)\partial_x u(\boldsymbol{\mu}, \boldsymbol{\xi}, x) = z(\boldsymbol{\mu}, x) \quad x \in (0, 1), \quad \boldsymbol{\xi} \in \boldsymbol{\Xi}$$
$$u(\boldsymbol{\mu}, \boldsymbol{\xi},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

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

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

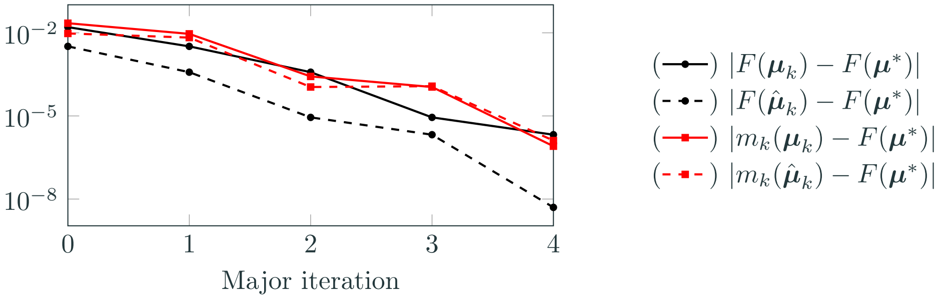
- **Parametrization:** $z(\boldsymbol{\mu}, x)$ – cubic splines with 51 knots, $n_{\boldsymbol{\mu}} = 53$

Optimal control and statistics



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

Global convergence without pointwise agreement

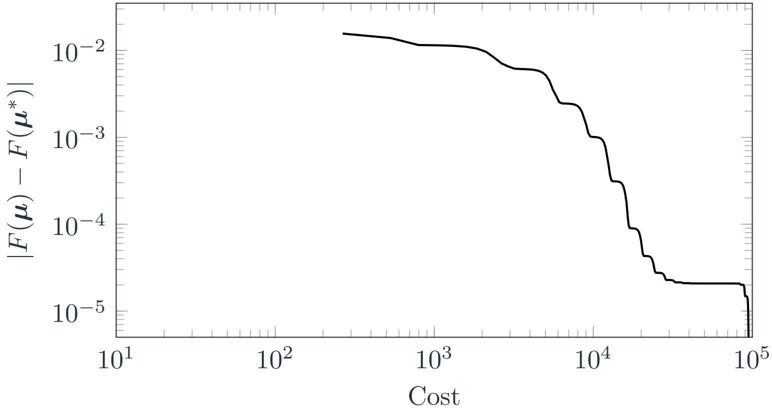


$F(\boldsymbol{\mu}_k)$	$m_k(\boldsymbol{\mu}_k)$	$F(\hat{\boldsymbol{\mu}}_k)$	$m_k(\hat{\boldsymbol{\mu}}_k)$	$\|\|\nabla F(\boldsymbol{\mu}_k)\|\|$	ρ_k	Success?
6.6506e-02	7.2694e-02	5.3655e-02	5.9922e-02	2.2959e-02	1.0257e+00	1.0000e+00
5.3655e-02	5.9593e-02	5.0783e-02	5.7152e-02	2.3424e-03	9.7512e-01	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 $\tau = 1$ ( ), $\tau = 10$ ( ), $\tau = 100$ ( ), $\tau = \infty$ ( )

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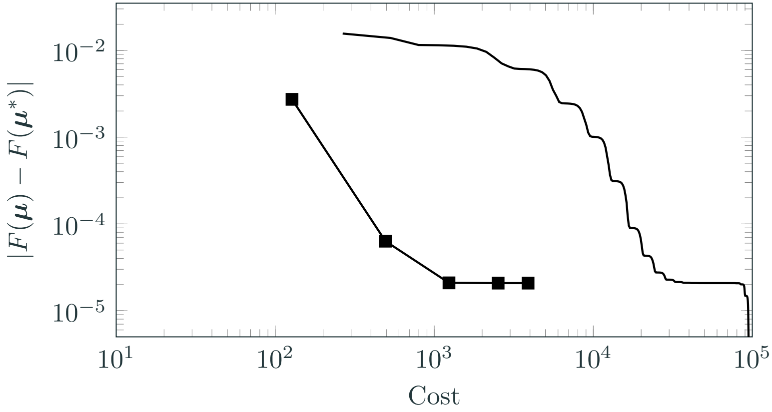

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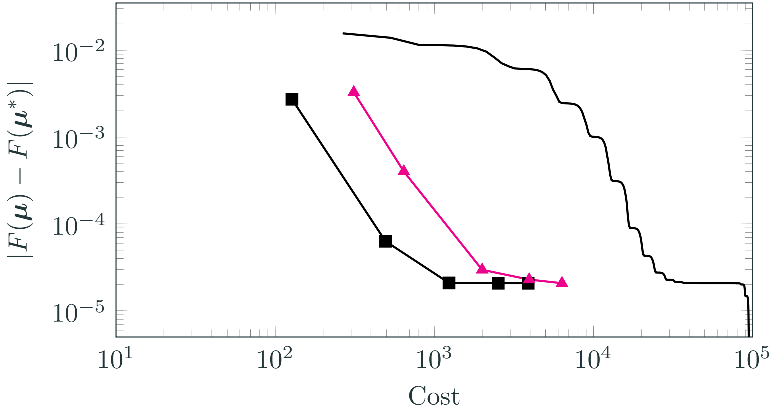

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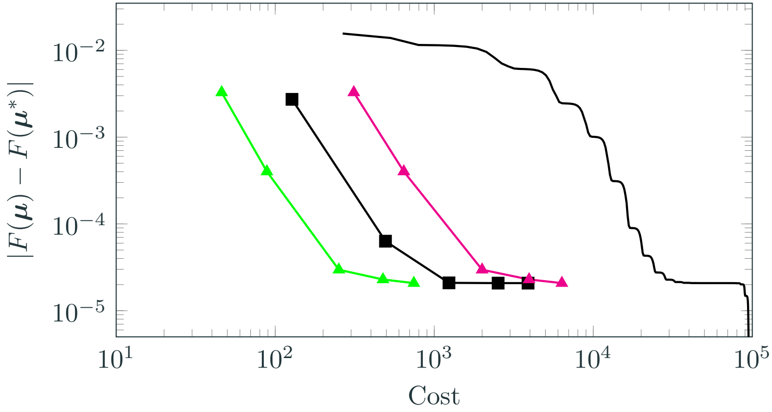

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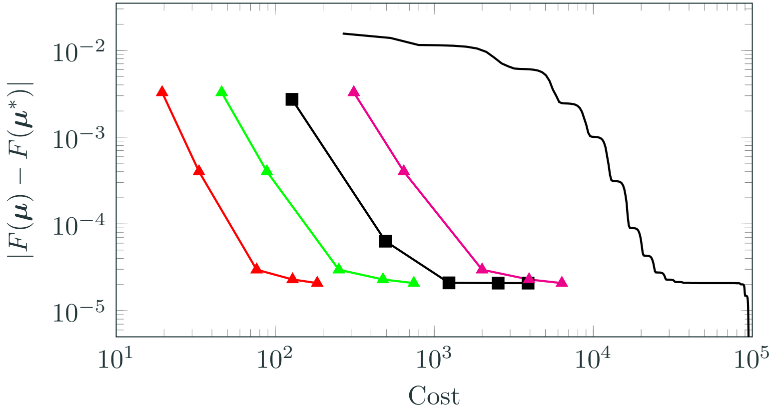
Significant reduction in cost, even if (largest) ROM only $10\times$ faster than HDM

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



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

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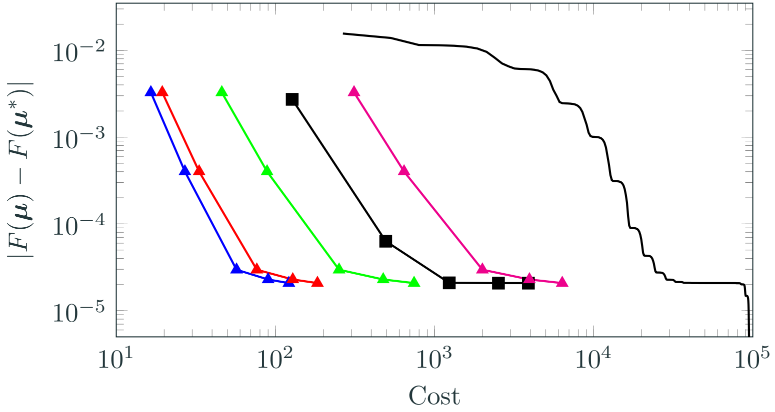
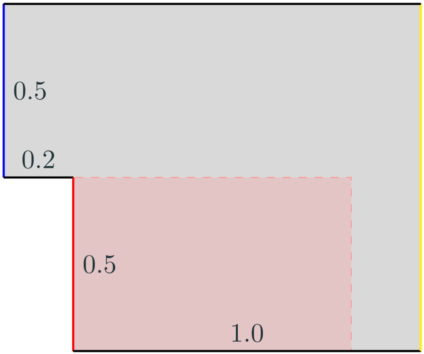
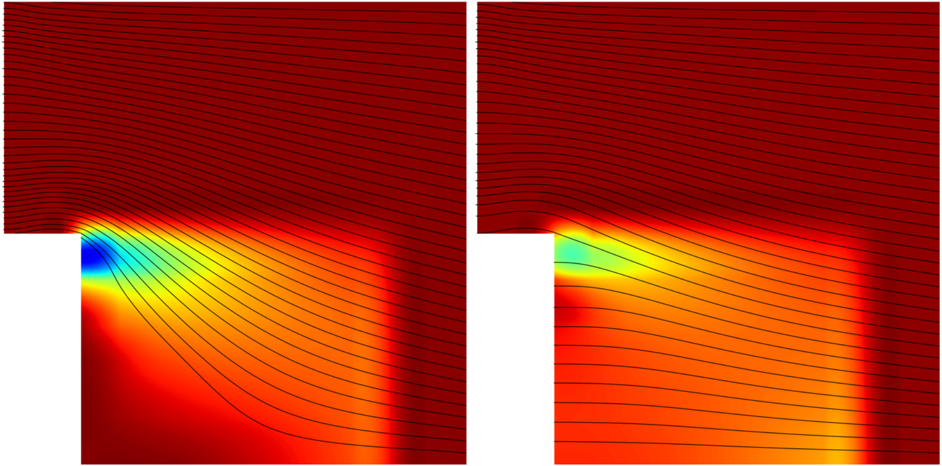


5-level isotropic SG (——), dimension-adaptive SG [Kouri et al., 2014] (——), and proposed ROM/SG for $\tau = 1$ (—▲—), $\tau = 10$ (—▲—), $\tau = 100$ (—▲—), $\tau = \infty$ (—▲—)

Backward facing step: minimize recirculation



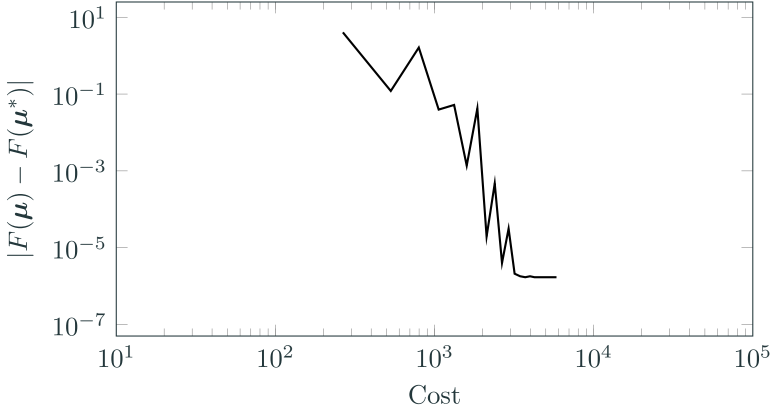
Geometry and boundary conditions for backward facing step. Boundary conditions: viscous wall (——), parametrized inflow($\boldsymbol{\mu}$) (——), stochastic inflow($\boldsymbol{\xi}$) (——), outflow (——). Vorticity magnitude minimized in red shaded region.



Mean vorticity corresponding to no inflow (left) and optimal inflow (right) along parametrized boundary.

Significant reduction in cost, if ROM only $10\times$ 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 (——) and proposed ROM/SG for $\tau = 1$ ( ), $\tau = 10$ ( ), $\tau = 100$ ( ), $\tau = \infty$ ( )

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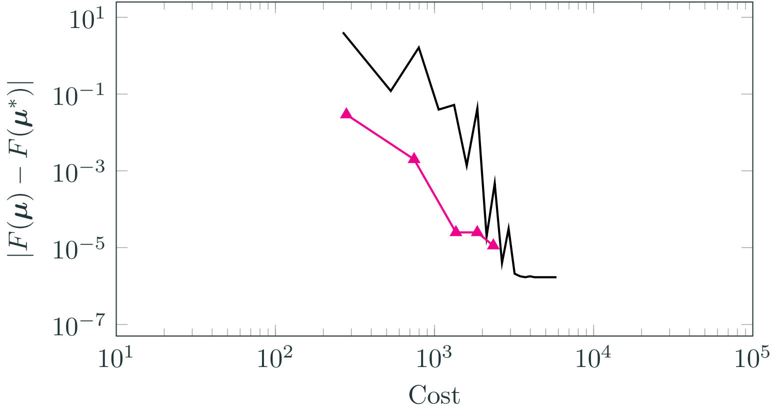

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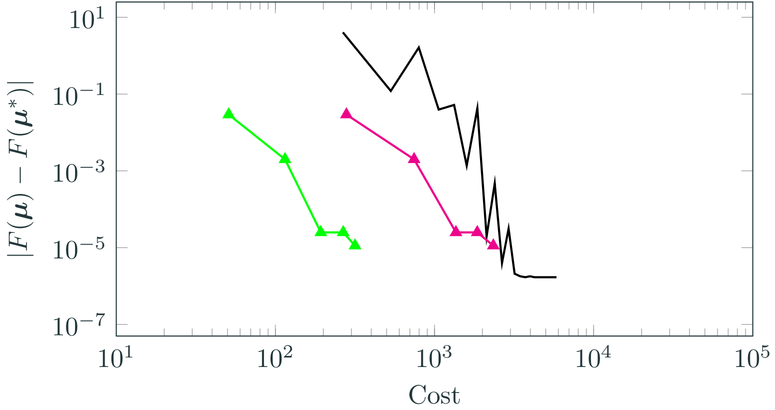

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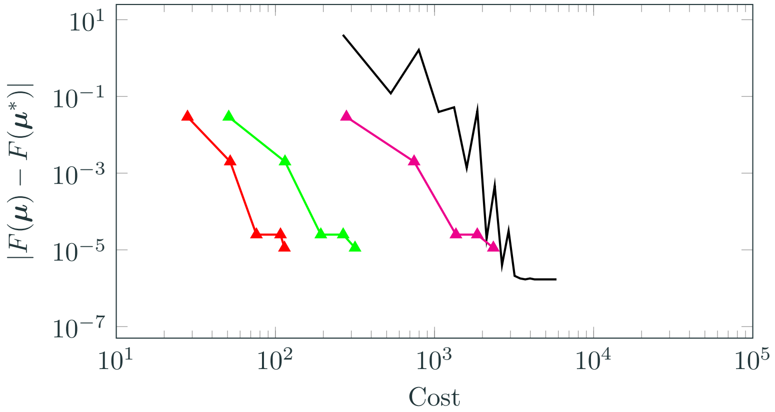

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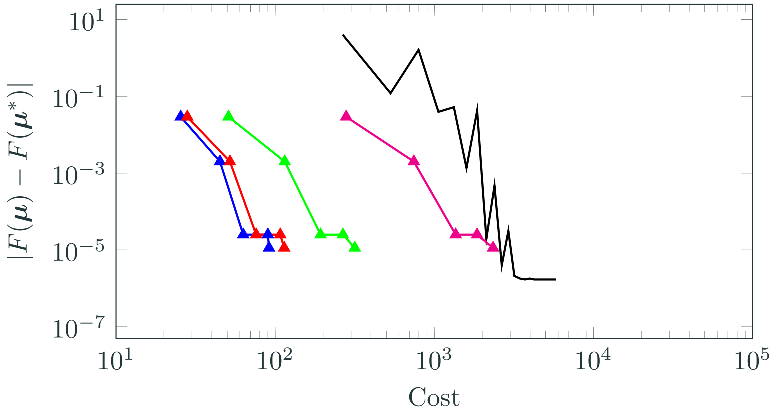
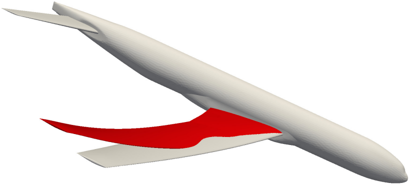
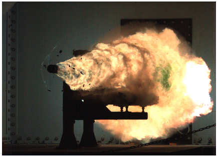


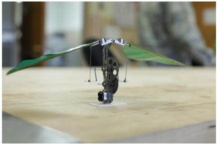
5-level isotropic SG (——) and proposed ROM/SG for $\tau = 1$ (—▲—), $\tau = 10$ (—▲—), $\tau = 100$ (—▲—), $\tau = \infty$ (—▲—)

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







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A trust-region algorithm with adaptive stochastic collocation for pde optimization under uncertainty.

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In *Frontiers in PDE-Constrained Optimization*. Springer.

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]

Energetically optimal flapping motions

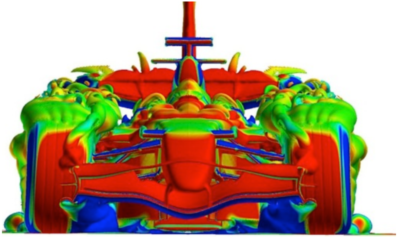
Energy = 9.4096e+00	Energy = 4.9476e+00	Energy = 4.6110e+00
Thrust = 1.7660e-01	Thrust = 2.5000e+00	Thrust = 2.5000e+00
Initial	Optimal Control	Optimal Shape/Control

[?], [?]

Deterministic PDE-constrained optimization formulation

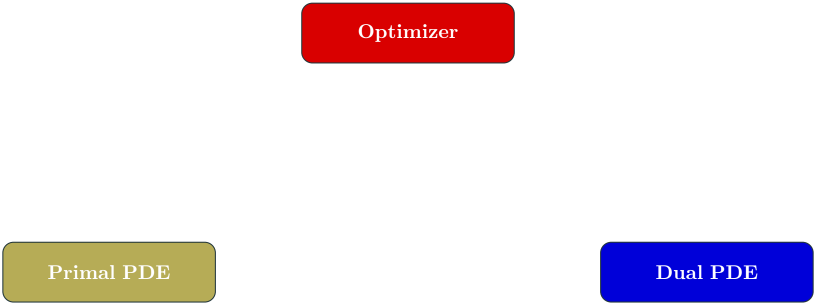
$$\begin{aligned} \underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathcal{J}(\boldsymbol{u}, \boldsymbol{\mu}) \\ \text{subject to} \quad & \boldsymbol{r}(\boldsymbol{u}; \boldsymbol{\mu}) = 0 \end{aligned}$$

- $\boldsymbol{r} : \mathbb{R}^{n_{\boldsymbol{u}}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \rightarrow \mathbb{R}^{n_{\boldsymbol{u}}}$ 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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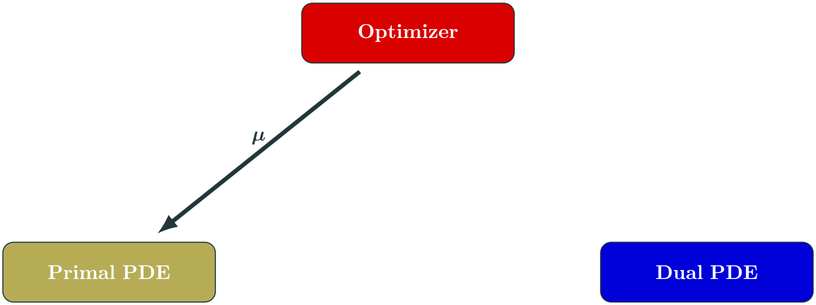

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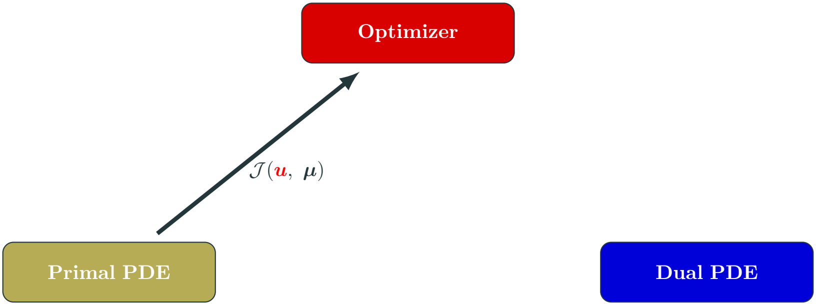

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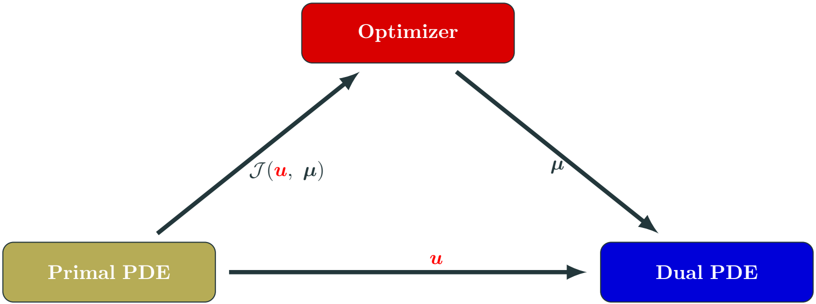

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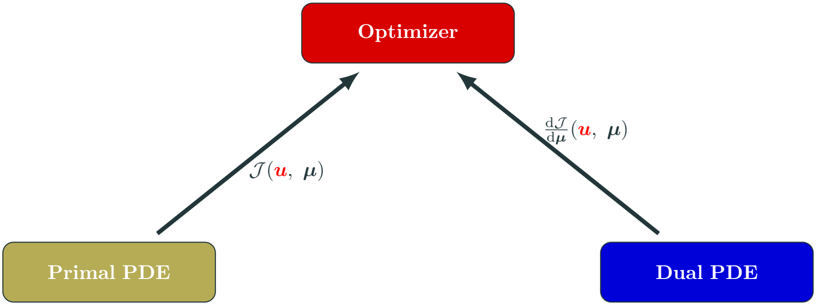


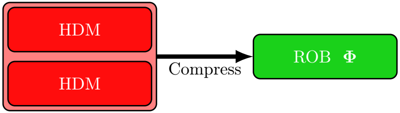
Trust region framework for optimization with ROMs

Schematic

μ-space

Breakdown of Computational Effort

Trust region framework for optimization with ROMs



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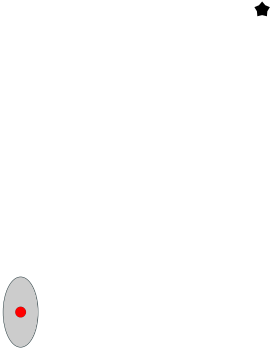

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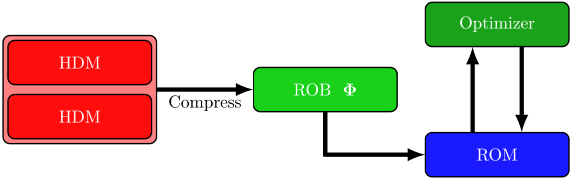

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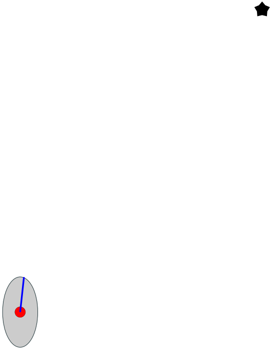

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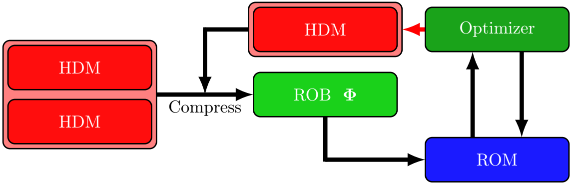

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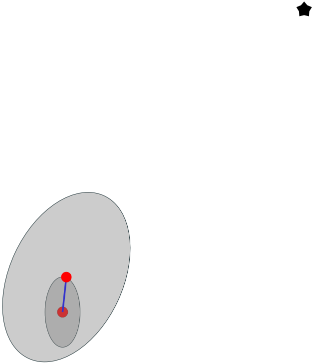

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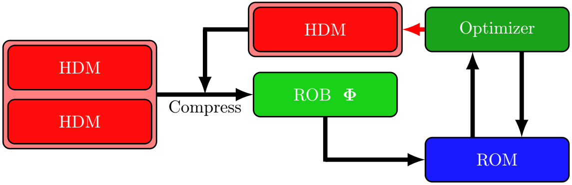

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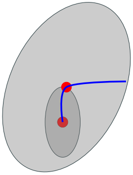

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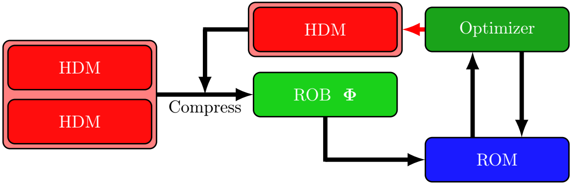

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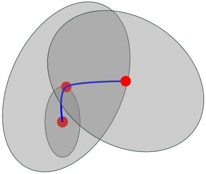

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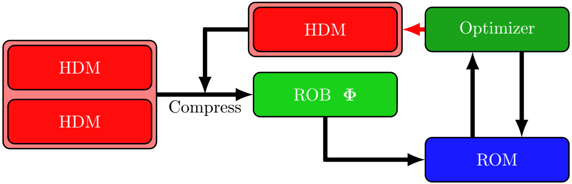

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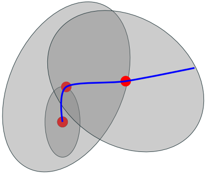

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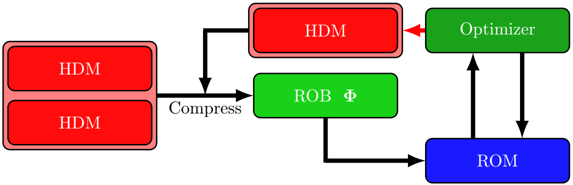

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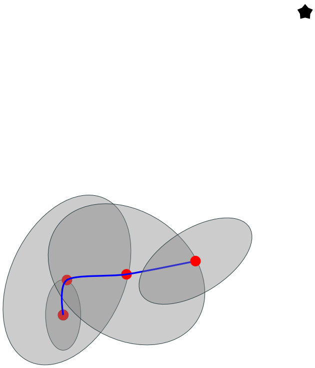

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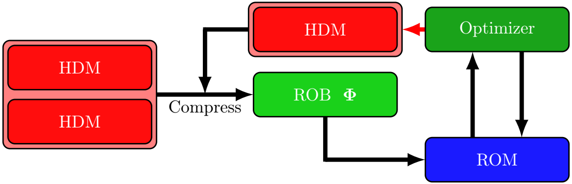

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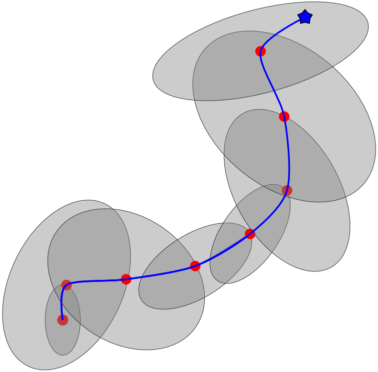

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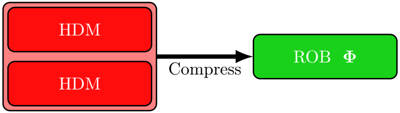

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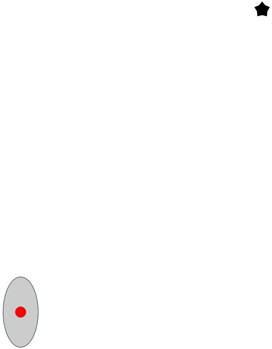

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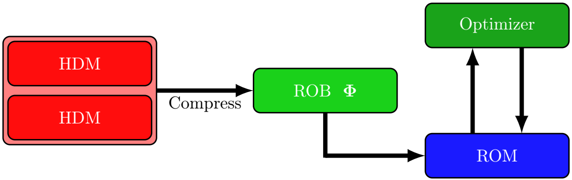

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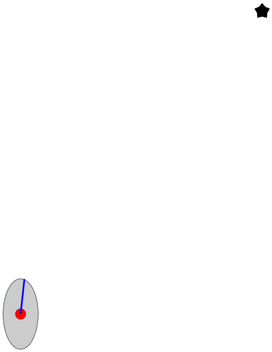

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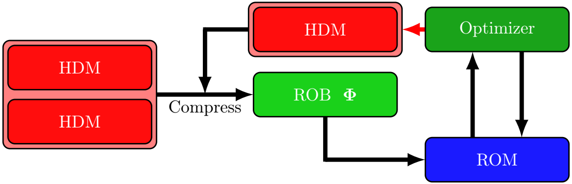

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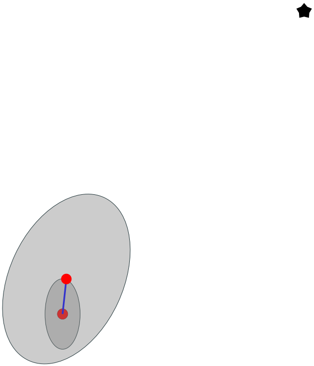

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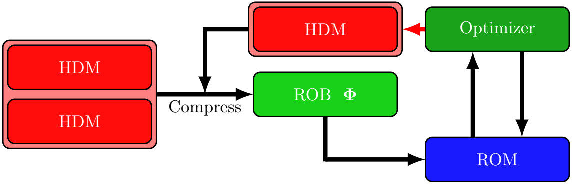

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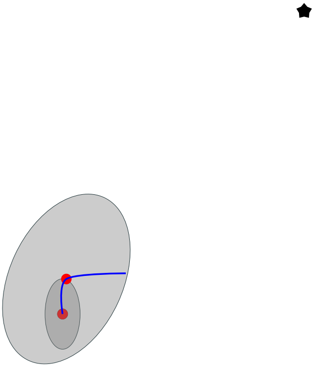

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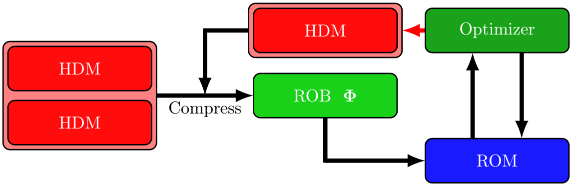

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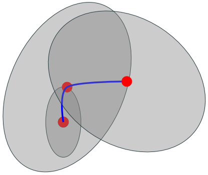

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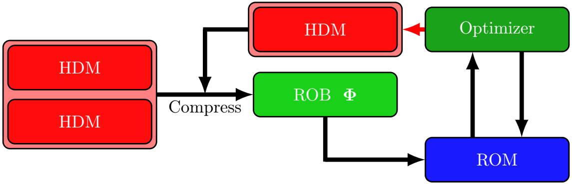

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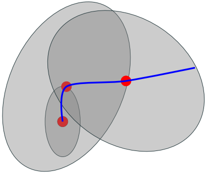

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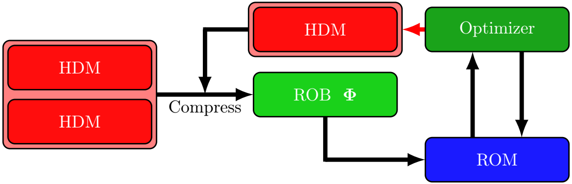

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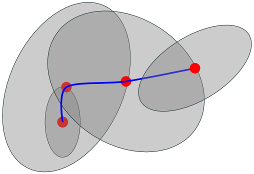

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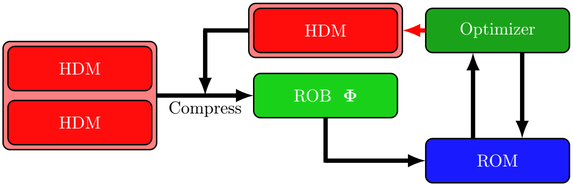

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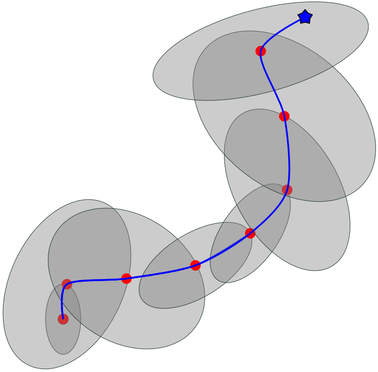

μ-space

Breakdown of Computational Effort

Relationship between the objective function and model

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**

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**

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*

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

Manage inexactness with trust region method

- Embedded in globally convergent **trust region** method
- **Error indicators**[2] to account for *all* sources of inexactness
- **Refinement** of approximation model using *greedy algorithms*

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

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

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

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

3: **Step acceptance**: Compute 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

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

Adaptivity

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

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

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

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