Efficient PDE Optimization under Uncertainty using Adaptive Model Reduction and Sparse Grids

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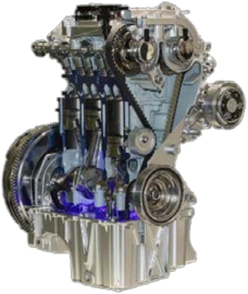
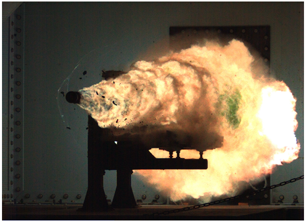
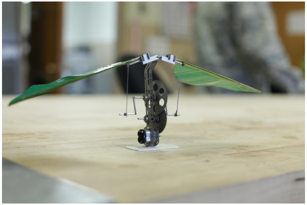
Current interest in computational physics reaches far beyond analysis of a single configuration of a physical system into ***design*** *(shape and topology) and* ***control*** *in an* ***uncertain*** *setting*



Engine System



EM Launcher



Micro-Aerial Vehicle

PDE-constrained optimization formulation

Goal: Rapidly solve PDE-constrained optimization problem of the form

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

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

Virtually all expense emanates from primal/dual PDE solvers

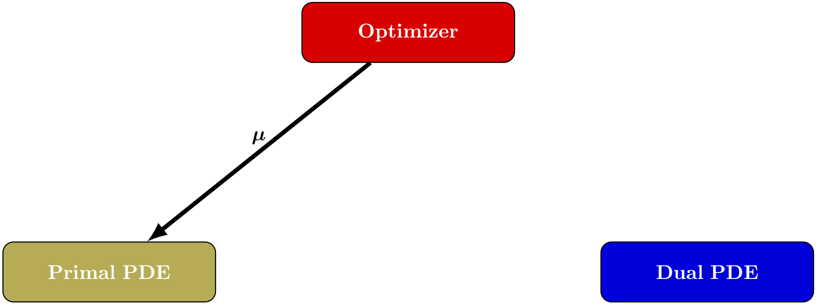
Optimizer

Primal PDE

Dual PDE

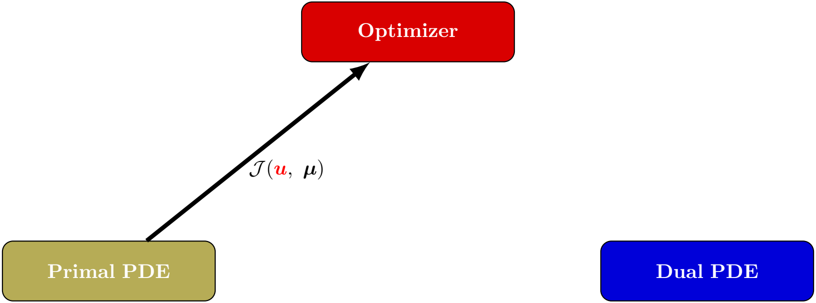
Nested approach to PDE-constrained optimization

Virtually all expense emanates from primal/dual PDE solvers



Nested approach to PDE-constrained optimization

Virtually all expense emanates from primal/dual PDE solvers



Nested approach to PDE-constrained optimization

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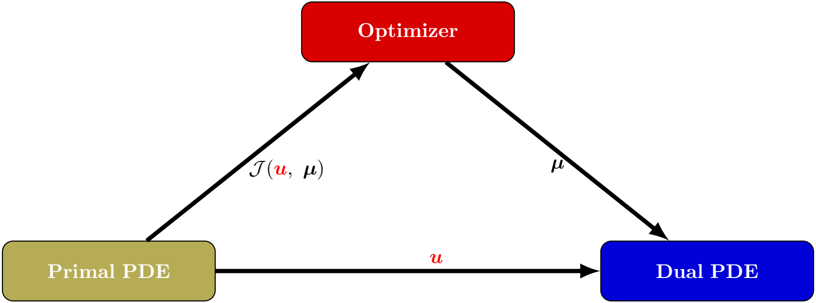

Nested approach to PDE-constrained optimization

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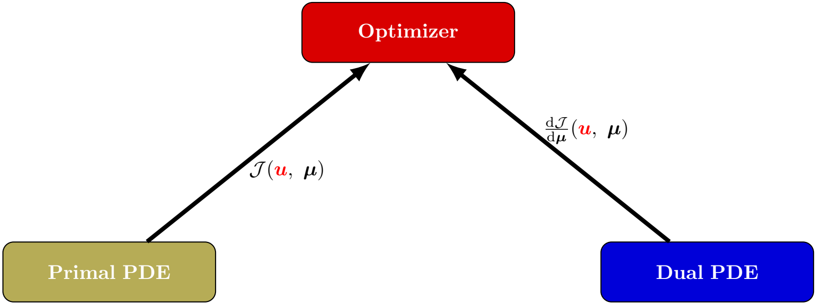


Maximum lift-to-drag airfoil configuration

Maximum stiffness lacrosse head

Optimal control based on compressible Navier-Stokes

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., 2016]

PDE-constrained optimization under uncertainty

Goal: Efficiently solve stochastic PDE-constrained optimization problems

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

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

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

Proposed approach: managed two-level inexactness

Two levels of inexactness to obtain an inexpensive, approximate version of the stochastic optimization problem

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

Manage inexactness with trust-region-like method

- Embedded in globally convergent **trust-region-like** algorithm with a strong connection to error indicators and refinement mechanism
- **Error indicators** to account for *both* sources of inexactness
- **Refinement** of integral approximation and reduced-order model via *dimension-adaptive* sparse grids and a *greedy method* over collocation nodes

Anisotropic sparse grids [Gerstner and Griebel, 2003]

1D Quadrature Rules: Define the difference operator

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

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

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

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

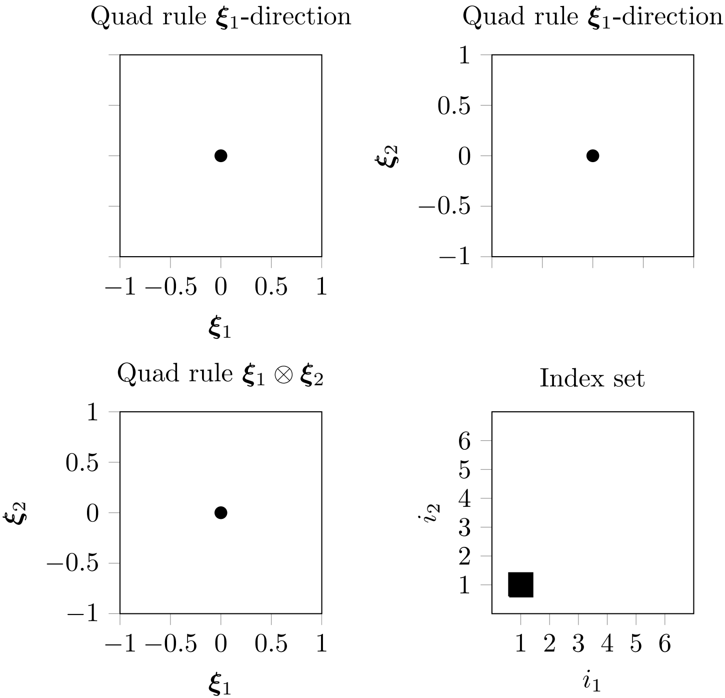
Forward Neighbors:

$$\mathcal{N}(\mathcal{I}) = \{\mathbf{k} + \mathbf{e}_j \mid \mathbf{k} \in \mathcal{I}\} \setminus \mathcal{I}$$

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

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

Tensor product quadrature



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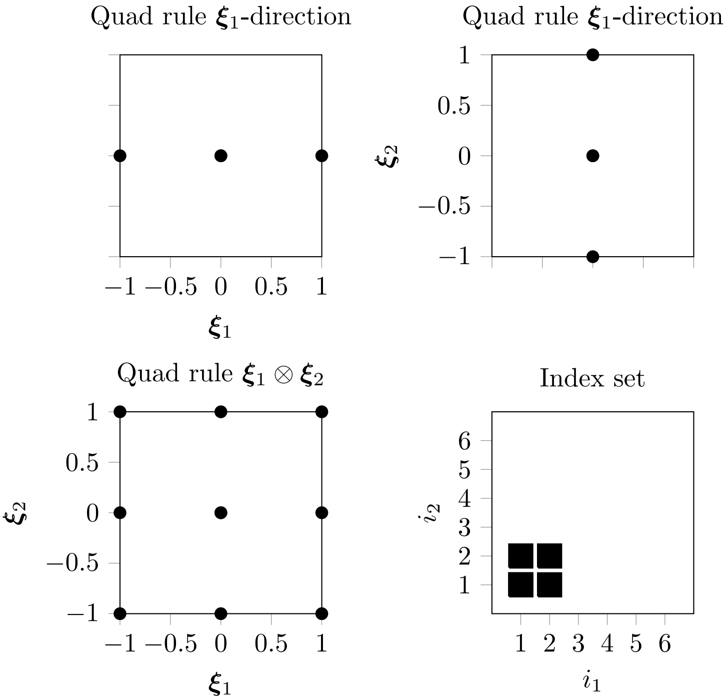

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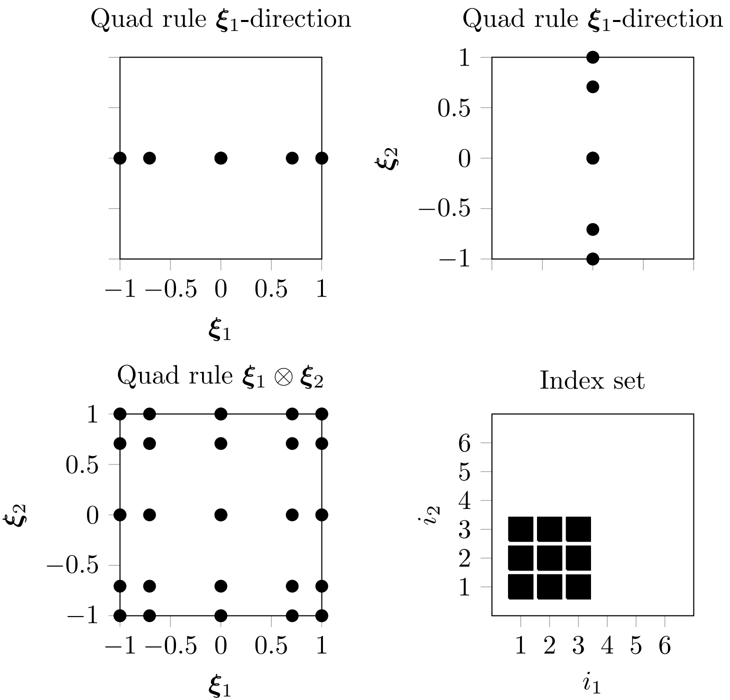

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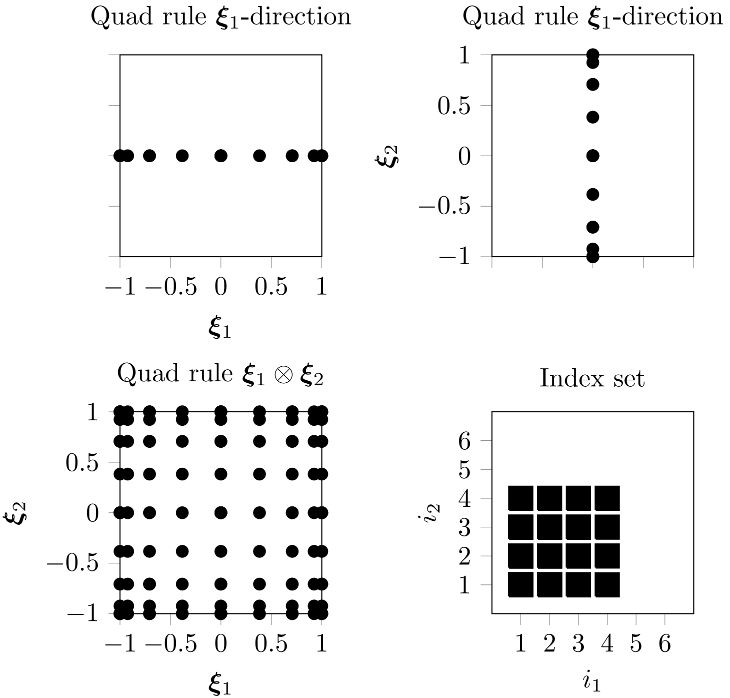

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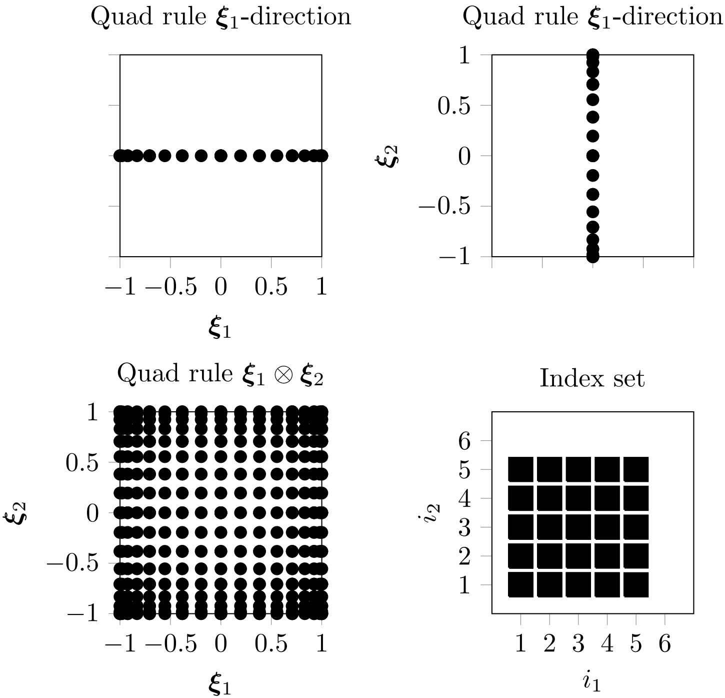
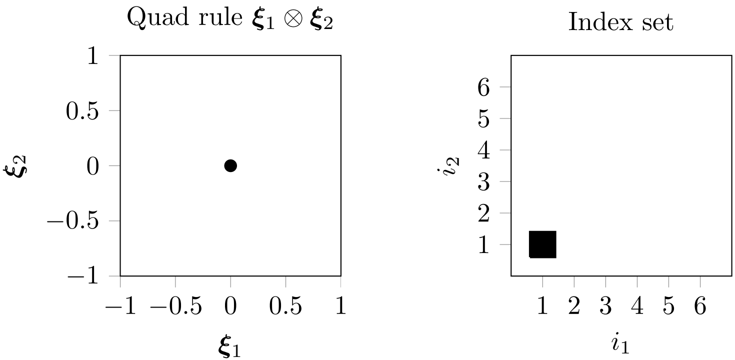


Isotropic sparse grid quadrature



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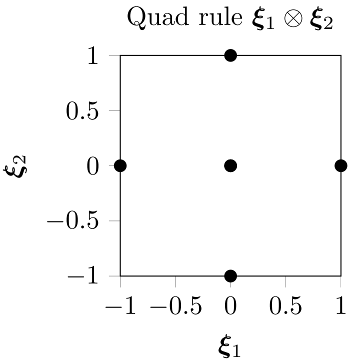

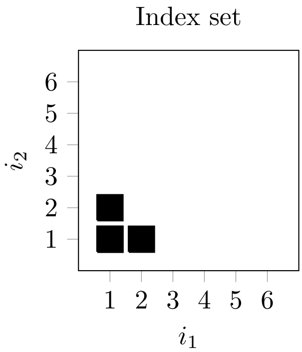

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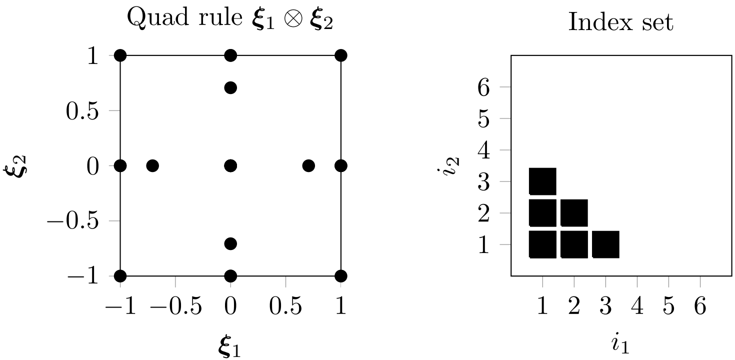

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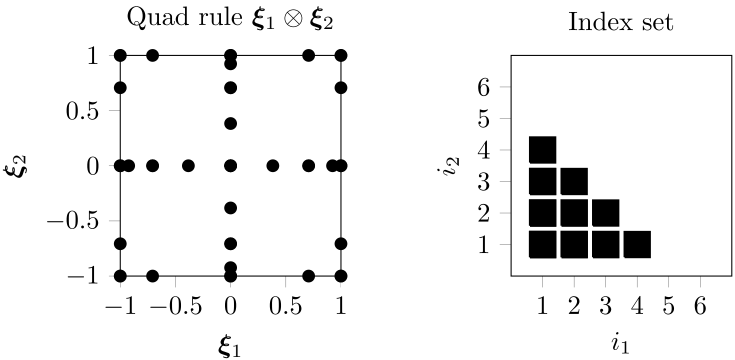

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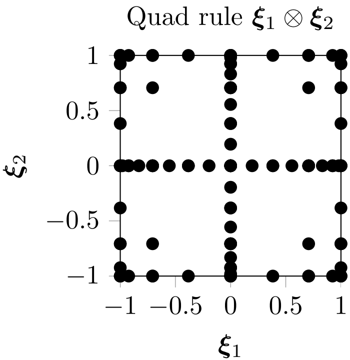

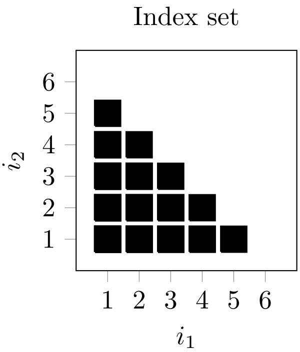

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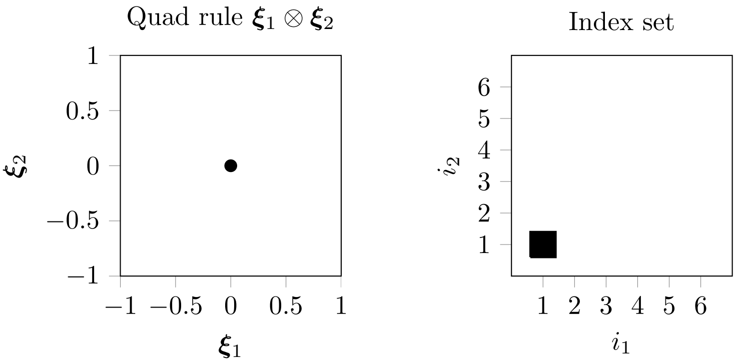

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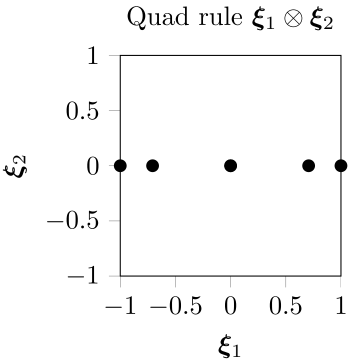

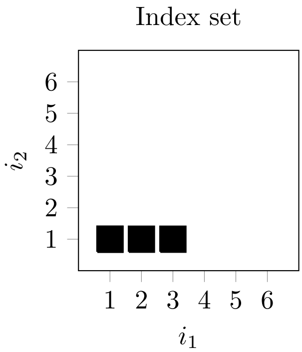

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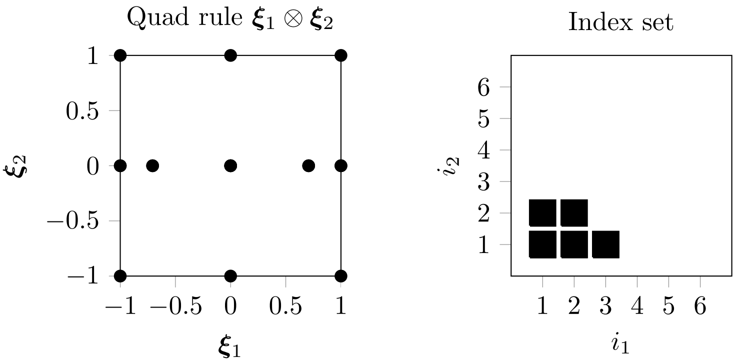

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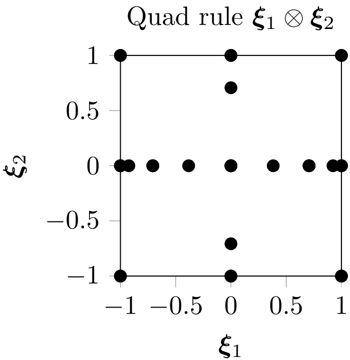

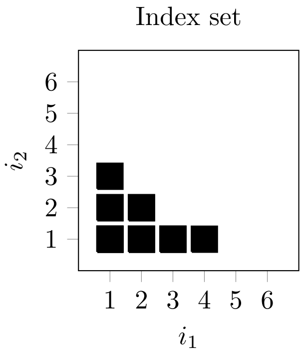

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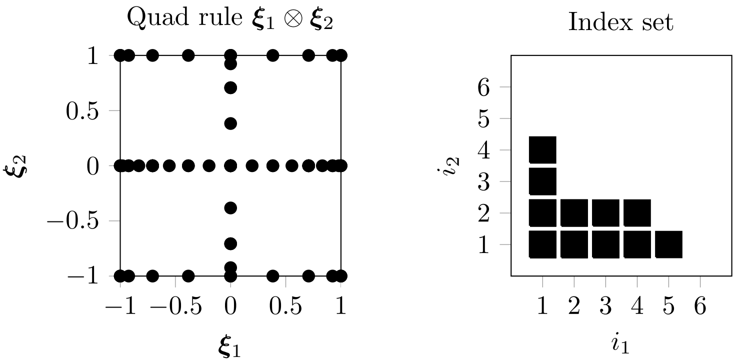
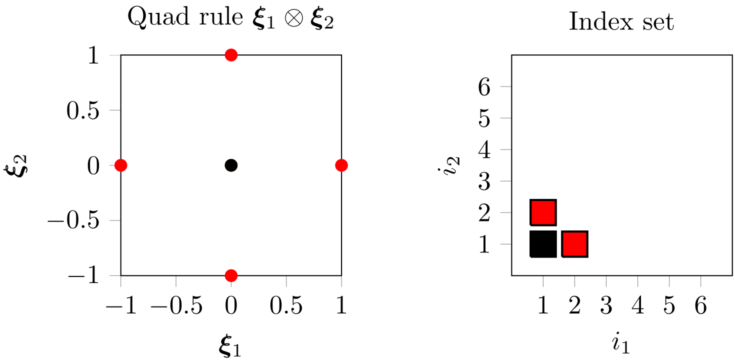
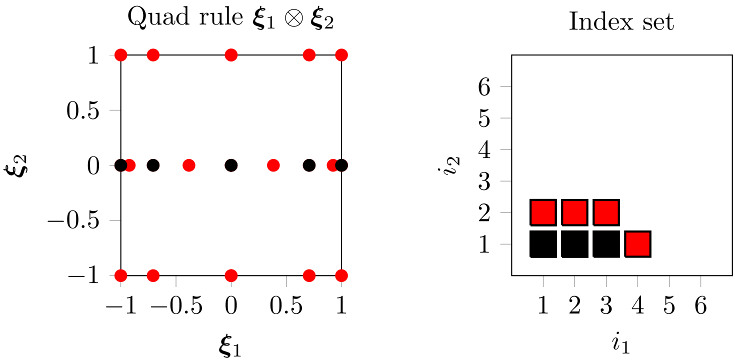


Anisotropic sparse grid quadrature: neighbors

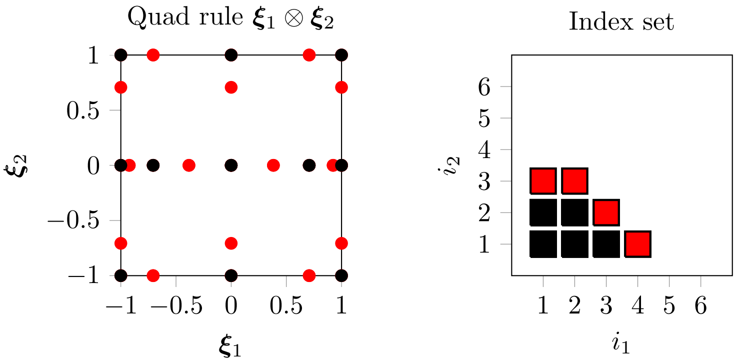


Index set ($\mathcal{I}$) – ● Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

Anisotropic sparse grid quadrature: neighbors

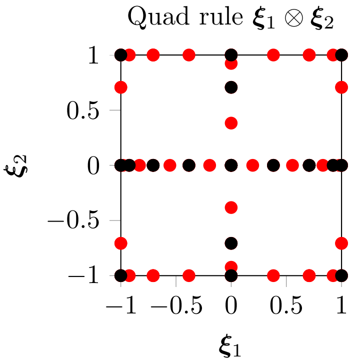


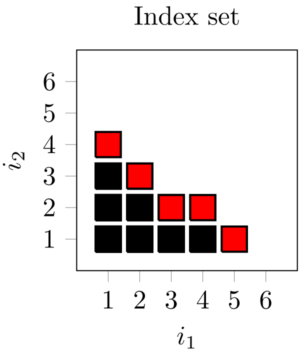
Index set ($\mathcal{I}$) – ●   Neighbors ($\mathcal{N}(\mathcal{I})$) – ●



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

Anisotropic sparse grid quadrature: neighbors





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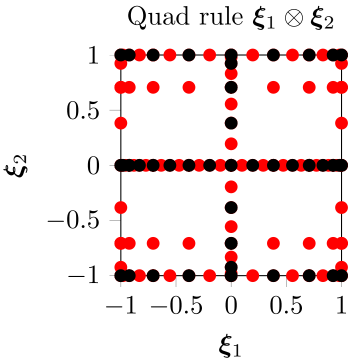
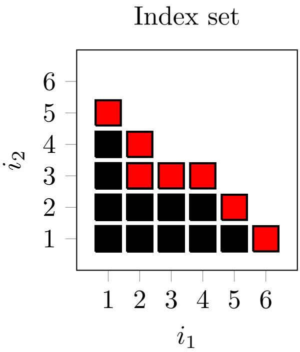




Index set ($\mathcal{I}$) – ● Neighbors ($\mathcal{N}(\mathcal{I})$) – ●

Stochastic collocation via anisotropic sparse grids

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

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

$$\Downarrow$$

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

Projection-based model reduction to reduce PDE size

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

$$\boldsymbol{u} \approx \boldsymbol{\Phi} \boldsymbol{y} \qquad \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\mu}} \approx \boldsymbol{\Phi} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{\mu}}$$

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

- Substitute assumption into high-dimensional model $\boldsymbol{r}(\boldsymbol{u},\, \boldsymbol{\mu},\, \boldsymbol{\xi}) = 0$ and use Galerkin projection to obtain a square system

$$\boldsymbol{\Phi}^T \boldsymbol{r}(\boldsymbol{\Phi} \boldsymbol{y},\, \boldsymbol{\mu},\, \boldsymbol{\xi}) = 0$$

Definition of $\boldsymbol{\Phi}$: data-driven reduction

State-Sensitivity Proper Orthogonal Decomposition (SSPOD)

- Collect state and sensitivity snapshots by sampling HDM

$$\begin{aligned} \boldsymbol{X} &= \begin{bmatrix} \boldsymbol{u}(\boldsymbol{\mu}_1,\, \boldsymbol{\xi}_1) & \boldsymbol{u}(\boldsymbol{\mu}_2,\, \boldsymbol{\xi}_2) & \cdots & \boldsymbol{u}(\boldsymbol{\mu}_n,\, \boldsymbol{\xi}_n) \end{bmatrix} \\ \boldsymbol{Y} &= \begin{bmatrix} \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_1,\, \boldsymbol{\xi}_1) & \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_2,\, \boldsymbol{\xi}_2) & \cdots & \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}_n,\, \boldsymbol{\xi}_n) \end{bmatrix} \end{aligned}$$

- Use Proper Orthogonal Decomposition to generate reduced basis for each individually

$$\begin{aligned} \boldsymbol{\Phi}_{\boldsymbol{X}} &= \mathrm{POD}(\boldsymbol{X}) \\ \boldsymbol{\Phi}_{\boldsymbol{Y}} &= \mathrm{POD}(\boldsymbol{Y}) \end{aligned}$$

- Concatenate and orthogonalize to get reduced-order basis

$$\boldsymbol{\Phi} = \mathrm{QR}\left(\begin{bmatrix} \boldsymbol{\Phi}_{\boldsymbol{X}} & \boldsymbol{\Phi}_{\boldsymbol{Y}} \end{bmatrix}\right)$$

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

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

$$\Downarrow$$

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

$$\Downarrow$$

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

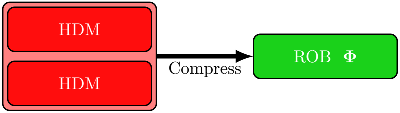
Trust-region framework for optimization

Schematic

$\boldsymbol{\mu}$-space

Breakdown of Computational Effort

Trust-region framework for optimization



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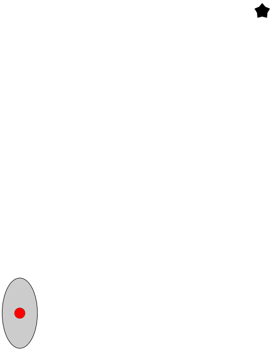

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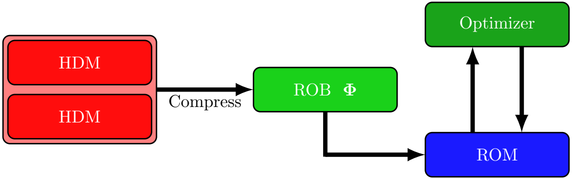

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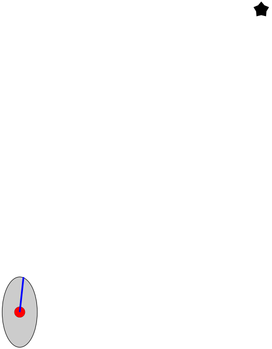

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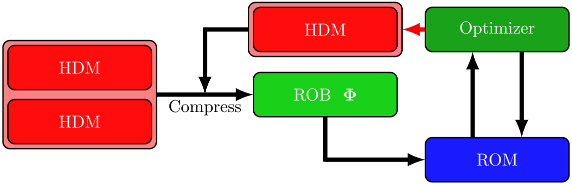

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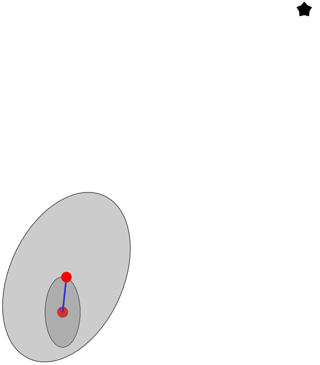

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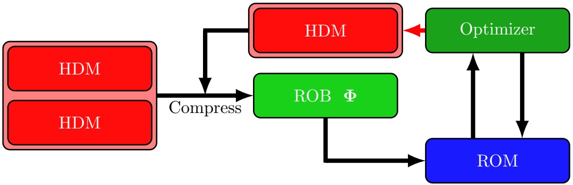

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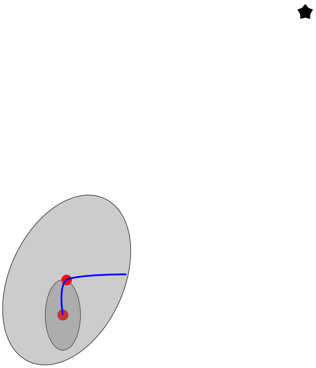

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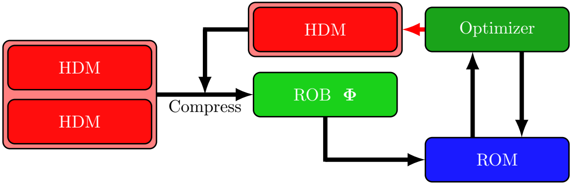

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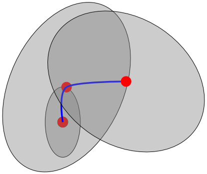

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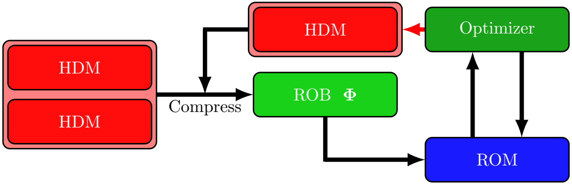
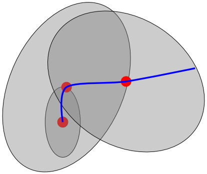
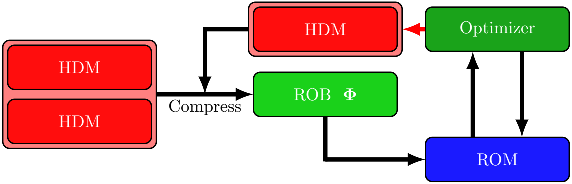


Schematic

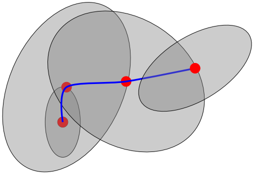


$\boldsymbol{\mu}$-space

Breakdown of Computational Effort



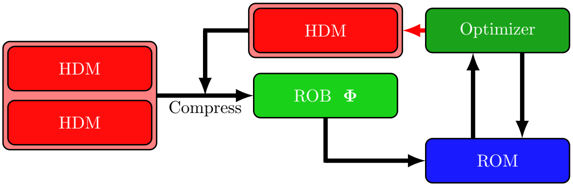
Schematic



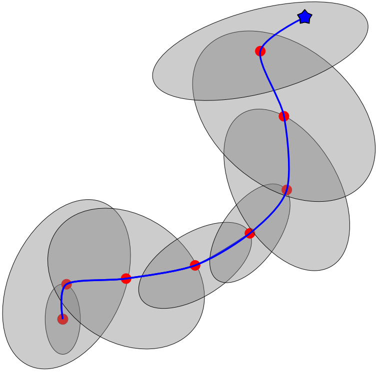
$\boldsymbol{\mu}$-space

Breakdown of Computational Effort

Trust-region framework for optimization



Schematic



$\boldsymbol{\mu}$-space

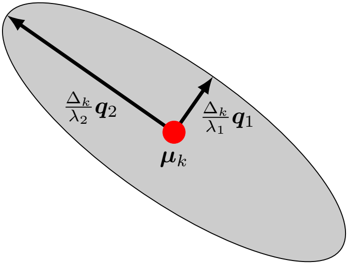
Breakdown of Computational Effort

Trust-regions based on error indicators: motivation

Let $\boldsymbol{\vartheta}_k(\boldsymbol{\mu})$ be a vector-valued error indicator, then to first order[1]

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

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



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

[1] assuming $\boldsymbol{\vartheta}_k(\boldsymbol{\mu}_k) = 0$, i.e., exactness at trust-region center

A trust-region method based on error indicators

Propose a trust-region method to solve the unconstrained optimization problem

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

that leverages trust-region subproblems of the form

$$\begin{aligned} \underset{\boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & m_k(\boldsymbol{\mu}) \\ \text{subject to} \quad & \vartheta_k(\boldsymbol{\mu}) \leq \Delta_k, \end{aligned}$$

where $\vartheta_k(\boldsymbol{\mu})$ is an *error bound*, i.e.,

there exists a constant[2] $\zeta > 0$ such that

$$|F(\boldsymbol{\mu}) - m_k(\boldsymbol{\mu})| \leq \zeta \vartheta_k(\boldsymbol{\mu})$$

[2] arbitrary, i.e., not tied to algorithmic parameters, and does not need to be computed or estimated

Trust-region model: two-level approximation based on reduced-order models and sparse grids

The trust-region subproblem

$$\begin{aligned} \underset{\boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & m_k(\boldsymbol{\mu}) \\ \text{subject to} \quad & \vartheta_k(\boldsymbol{\mu}) \leq \Delta_k, \end{aligned}$$

is defined as

$$\begin{aligned} m_k(\boldsymbol{\mu}) &= \mathbb{E}_{\mathcal{I}_k}\left[\mathcal{J}(\boldsymbol{\Phi}_k \boldsymbol{y}(\boldsymbol{\mu},\,\cdot\,),\, \boldsymbol{\mu},\,\cdot\,)\right] \\ \vartheta_k(\boldsymbol{\mu}) &= \alpha_1 \mathbb{E}_{\mathcal{I}_k \cup \mathcal{N}(\mathcal{I}_k)}\left[\left|\left|\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{y}(\boldsymbol{\mu},\,\cdot\,);\, \boldsymbol{\mu},\,\cdot\,)\right|\right|\right] + \\ &\quad\; \alpha_2 \left|\mathbb{E}_{\mathcal{N}(\mathcal{I}_k)}\left[\mathcal{J}(\boldsymbol{\Phi}_k \boldsymbol{y}(\boldsymbol{\mu},\,\cdot\,),\, \boldsymbol{\mu},\,\cdot\,)\right]\right| \end{aligned}$$

An error indicator for the model gradient is also required and chosen as

$$\begin{aligned} \varphi_k = {} & \beta_1 \mathbb{E}_{\mathcal{I}_k \cup \mathcal{N}(\mathcal{I}_k)}\left[\left|\left|\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{y}(\boldsymbol{\mu}_k,\,\cdot);\, \boldsymbol{\mu}_k,\,\cdot\,)\right|\right|\right] + \\ & \beta_2 \mathbb{E}_{\mathcal{I}_k \cup \mathcal{N}(\mathcal{I}_k)}\left[\left|\left|\boldsymbol{r}^{\partial}(\boldsymbol{\Phi}_k \boldsymbol{y}(\boldsymbol{\mu}_k,\,\cdot);\, \boldsymbol{\mu}_k,\,\cdot\,)\right|\right|\right] + \\ & \beta_3 \left|\left|\mathbb{E}_{\mathcal{N}(\mathcal{I}_k)}\left[\nabla_{\boldsymbol{\mu}} \mathcal{J}(\boldsymbol{\Phi}_k \boldsymbol{y}(\boldsymbol{\mu}_k,\,\cdot\,),\, \boldsymbol{\mu}_k,\,\cdot\,)\right]\right|\right| \end{aligned}$$

Error indicator for function values must account for ROM inaccuracy and sparse grid truncation error

Error indicator for function values are based on collocation of the **residual norm** to account for ROM error and **forward neighbors** to account for truncation error

Define

$$\hat{\mathcal{J}}(\boldsymbol{\mu},\, \boldsymbol{\xi}) \equiv \mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu},\, \boldsymbol{\xi}),\, \boldsymbol{\mu},\, \boldsymbol{\xi}) \qquad \hat{\mathcal{J}}_r(\boldsymbol{\mu},\, \boldsymbol{\xi}) \equiv \mathcal{J}(\boldsymbol{\Phi} \boldsymbol{y}(\boldsymbol{\mu},\, \boldsymbol{\xi}),\, \boldsymbol{\mu},\, \boldsymbol{\xi})$$

$$\hat{\boldsymbol{r}}_r(\boldsymbol{\mu},\, \boldsymbol{\xi}) \equiv \boldsymbol{r}(\boldsymbol{\Phi} \boldsymbol{y}(\boldsymbol{\mu},\, \boldsymbol{\xi}),\, \boldsymbol{\mu},\, \boldsymbol{\xi})$$

$$\begin{aligned}\left|\mathbb{E}\left[\hat{\mathcal{J}}(\boldsymbol{\mu},\,\cdot\,)\right] - \mathbb{E}_{\mathcal{I}}\left[\hat{\mathcal{J}}_r(\boldsymbol{\mu},\,\cdot\,)\right]\right| &\leq \mathbb{E}\left[\left|\hat{\mathcal{J}}(\boldsymbol{\mu},\,\cdot\,) - \hat{\mathcal{J}}_r(\boldsymbol{\mu},\,\cdot\,)\right|\right] + \left|\mathbb{E}_{\mathcal{I}^c}\left[\hat{\mathcal{J}}_r(\boldsymbol{\mu},\,\cdot\,)\right]\right| \\ &\lesssim \zeta_1 \mathbb{E}_{\mathcal{I} \cup \mathcal{N}(\mathcal{I})}\left[|||\hat{\boldsymbol{r}}_r(\boldsymbol{\mu},\, \boldsymbol{\xi})|||\right] + \left|\mathbb{E}_{\mathcal{N}(\mathcal{I})}\left[\hat{\mathcal{J}}_r(\boldsymbol{\mu},\,\cdot\,)\right]\right|\end{aligned}$$

Error indicator for gradients must account for primal and dual ROM inaccuracy and sparse grid truncation error

Error indicator for function gradients are based on collocation of the **primal and dual residual norm** to account for ROM error and **forward neighbors** to account for truncation error

Define

$$\hat{\boldsymbol{r}}_r^{\partial}(\boldsymbol{\mu},\,\boldsymbol{\xi}) \equiv \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}}(\boldsymbol{\Phi}\boldsymbol{y}(\boldsymbol{\mu},\ \boldsymbol{\xi}))\boldsymbol{\Phi}\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu},\ \boldsymbol{\xi}) + \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{\mu}}(\boldsymbol{\Phi}\boldsymbol{y}(\boldsymbol{\mu},\ \boldsymbol{\xi}),\ \boldsymbol{\mu},\,\boldsymbol{\xi})$$

$$\begin{aligned}
&\left\|\mathbb{E}\left[\nabla_{\boldsymbol{\mu}}\hat{\mathcal{J}}(\boldsymbol{\mu},\,\cdot\,)\right] - \mathbb{E}_{\mathcal{I}}\left[\nabla_{\boldsymbol{\mu}}\hat{\mathcal{J}}(\boldsymbol{\mu},\,\cdot\,)\right]\right\| \\
&\qquad \leq \mathbb{E}\left[\left\|\nabla_{\boldsymbol{\mu}}\hat{\mathcal{J}}(\boldsymbol{\mu},\,\cdot\,) - \nabla_{\boldsymbol{\mu}}\hat{\mathcal{J}}_r(\boldsymbol{\mu},\,\cdot\,)\right\|\right] + \left\|\mathbb{E}_{\mathcal{I}^c}\left[\nabla_{\boldsymbol{\mu}}\hat{\mathcal{J}}_r(\boldsymbol{\mu},\,\cdot\,)\right]\right\| \\
&\qquad \lesssim \zeta_2\mathbb{E}_{\mathcal{I}\cup\mathcal{N}(\mathcal{I})}\left[\|\hat{\boldsymbol{r}}_r(\boldsymbol{\mu},\,\cdot\,)\|\right] + \zeta_3\mathbb{E}_{\mathcal{I}\cup\mathcal{N}(\mathcal{I})}\left[\left\|\hat{\boldsymbol{r}}_r^{\partial}(\boldsymbol{\mu},\,\cdot\,)\right\|\right] + \left\|\mathbb{E}_{\mathcal{N}(\mathcal{I})}\left[\nabla_{\boldsymbol{\mu}}\hat{\mathcal{J}}_r(\boldsymbol{\mu},\,\cdot\,)\right]\right\|
\end{aligned}$$

Trust-region method based on error indicators: algorithm

1: **Model update**: Choose m_k, i.e., $\mathcal{I}_k$ and $\mathbf{\Phi}_k$, such that

$$\vartheta_k(\boldsymbol{\mu}_k) \leq \kappa_1 \Delta_k \qquad \varphi_k \quad \leq \kappa_2 \, ||\nabla m_k(\boldsymbol{\mu}_k)||$$

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

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

3: **Step acceptance**: Compute

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

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

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

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

Trust-region method based on error indicators: convergence

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

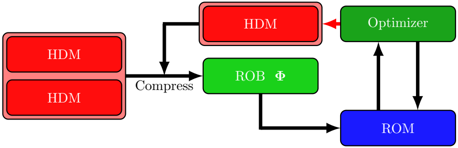
The trust-region method guarantees

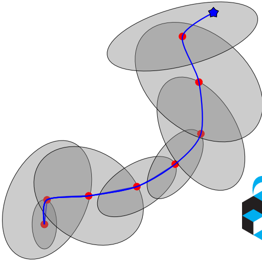
$$\boxed{\liminf_{k\to\infty} ||\nabla_{\boldsymbol{\mu}}\mathbb{E}\left[\mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu}_k,\,\cdot\,),\,\boldsymbol{\mu}_k,\,\cdot\,)\right]|| = 0}$$

if $\exists \zeta,\,\tau > 0$ such that

$$|\mathbb{E}\left[\mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu},\,\cdot\,)\,\boldsymbol{\mu},\,\cdot\,)\right] - \mathbb{E}\left[\mathcal{J}(\boldsymbol{\Phi}\boldsymbol{y}(\boldsymbol{\mu},\,\cdot\,)\,\boldsymbol{\mu},\,\cdot\,)\right]| \leq \zeta\vartheta_k(\boldsymbol{\mu})$$

$$||\nabla_{\boldsymbol{\mu}}\mathbb{E}\left[\mathcal{J}(\boldsymbol{u}(\boldsymbol{\mu}_k,\,\cdot\,),\,\boldsymbol{\mu}_k,\,\cdot\,)\right] - \nabla_{\boldsymbol{\mu}}\mathbb{E}\left[\mathcal{J}(\boldsymbol{\Phi}\boldsymbol{y}(\boldsymbol{\mu}_k,\,\cdot\,),\,\boldsymbol{\mu}_k,\,\cdot\,)\right]|| \leq \tau\varphi_k$$





Control two-level inexactness: dimension-adaptive sparse grids and greedy sampling

while $\left|\mathbb{E}_{\mathcal{N}(\mathcal{I}_k)}\left[\mathcal{J}(\boldsymbol{\Phi}\boldsymbol{y}(\boldsymbol{\mu},\,\cdot\,),\,\boldsymbol{\mu},\,\cdot\,)\right]\right| > \frac{1}{2\alpha_2}\kappa_1\Delta_k$ **do**

Refine index set: Let $\mathbf{j} = \underset{\mathbf{j}\in\mathcal{N}(\mathcal{I}_k)}{\arg\max}\left|\mathbb{E}_{\mathbf{j}}\left[\mathcal{J}(\boldsymbol{\Phi}\boldsymbol{y}(\boldsymbol{\mu},\,\cdot\,),\,\boldsymbol{\mu},\,\cdot\,)\right]\right|$

$$\mathcal{I}_k \leftarrow \mathcal{I}_k \cup \{\mathbf{j}\}$$

while $\mathbb{E}_{\mathcal{I}_k\cup\mathcal{N}(\mathcal{I}_k)}\left[||\boldsymbol{r}(\boldsymbol{\Phi}\boldsymbol{y}(\boldsymbol{\mu}_k,\,\cdot\,),\,\boldsymbol{\mu}_k,\,\cdot\,)||\right] > \frac{1}{2\alpha_1}\kappa_1\Delta_k$ **do**

Evaluate error indicator: For each $\boldsymbol{\xi}_j \in \boldsymbol{\Xi}_{\mathcal{I}_k\cup\mathcal{N}(\mathcal{I}_k)}$, compute

$$r_j = ||\boldsymbol{r}(\boldsymbol{\Phi}\boldsymbol{y}(\boldsymbol{\mu}_k,\,\boldsymbol{\xi}_j),\,\boldsymbol{\mu}_k,\,\boldsymbol{\xi}_j\,)||$$

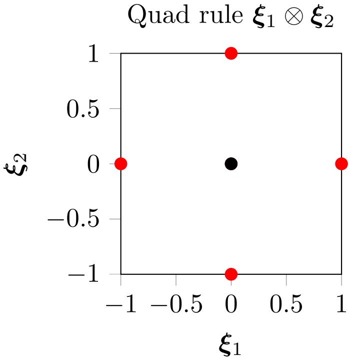
Sample high-dimensional model: Let $j^* = \arg\max r_j$ and compute

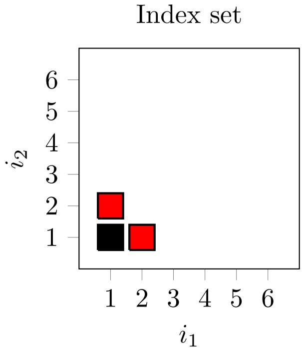
$$\boldsymbol{u}(\boldsymbol{\mu}_k,\boldsymbol{\xi}_{j^*}),\;\; \frac{\partial\boldsymbol{u}}{\partial\boldsymbol{\mu}}(\boldsymbol{\mu}_k,\boldsymbol{\xi}_{j^*})$$

and update reduced-order basis, $\boldsymbol{\Phi}_k$, using SSPOD

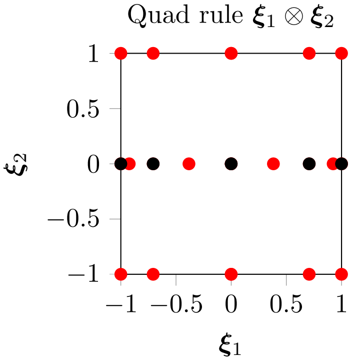
end while

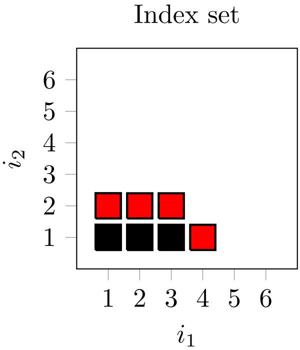
end while





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





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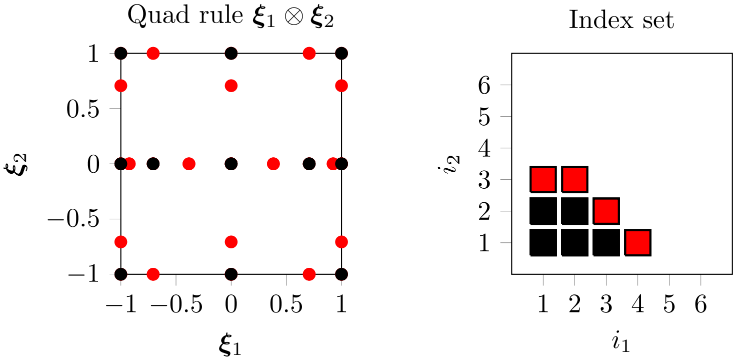

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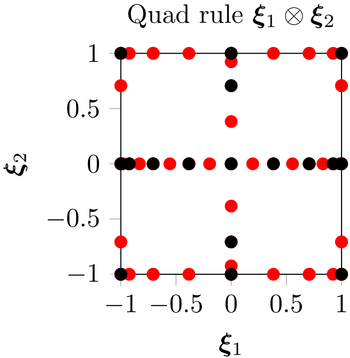

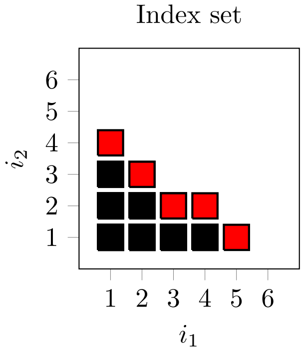

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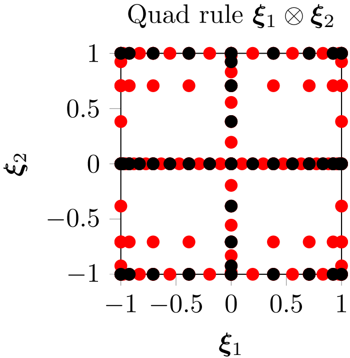
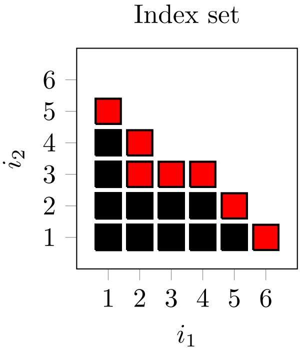




Index set ($\mathcal{I}$) – ●

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

Optimal control of steady Burgers' equation

- **Optimization problem:**

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

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

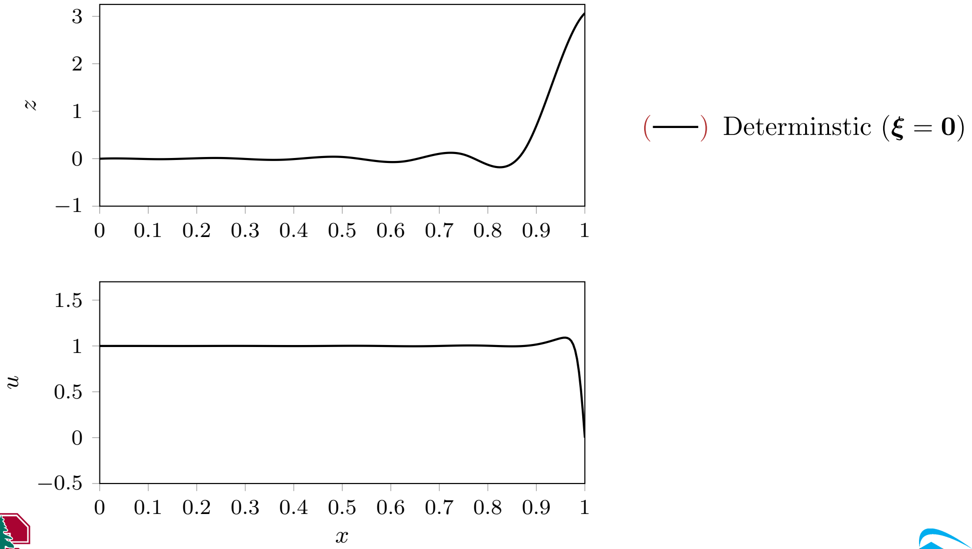
$$-\nu(\boldsymbol{\xi})\partial_{xx}u(\boldsymbol{\mu},\, \boldsymbol{\xi},\, x) + u(\boldsymbol{\mu},\, \boldsymbol{\xi},\, x)\partial_x u(\boldsymbol{\mu},\, \boldsymbol{\xi},\, x) = z(\boldsymbol{\mu},\, x) \quad x \in (0,\, 1), \quad \boldsymbol{\xi} \in \boldsymbol{\Xi}$$
$$u(\boldsymbol{\mu},\,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

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

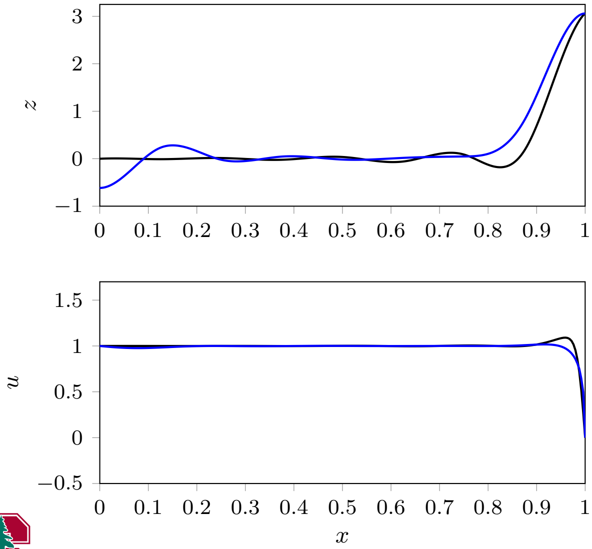
$$\nu(\boldsymbol{\xi}) = 10^{\xi_1 - 2} \qquad d_0(\boldsymbol{\xi}) = 1 + \frac{\xi_2}{1000} \qquad d_1(\boldsymbol{\xi}) = \frac{\xi_3}{1000}$$

- **Parametrization:** $z(\boldsymbol{\mu},\, x)$ – cubic splines with 9 knots, $n_{\boldsymbol{\mu}} = 11$

Trust-region method recovers optimal control and statistics



Trust-region method recovers optimal control and statistics

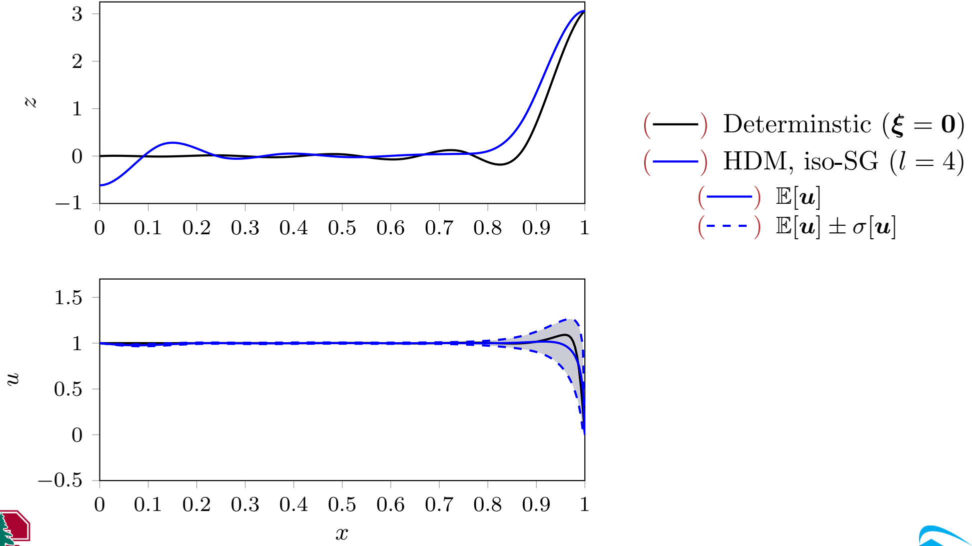


(——) Determinstic ($\boldsymbol{\xi} = \mathbf{0}$)

(——) HDM, iso-SG ($l = 4$)

(——) $\mathbb{E}[\boldsymbol{u}]$

Trust-region method recovers optimal control and statistics



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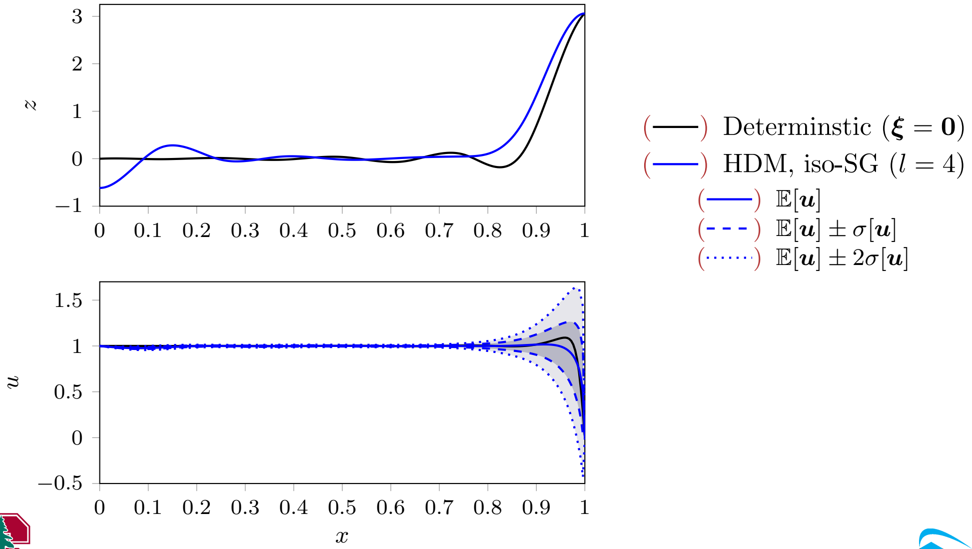

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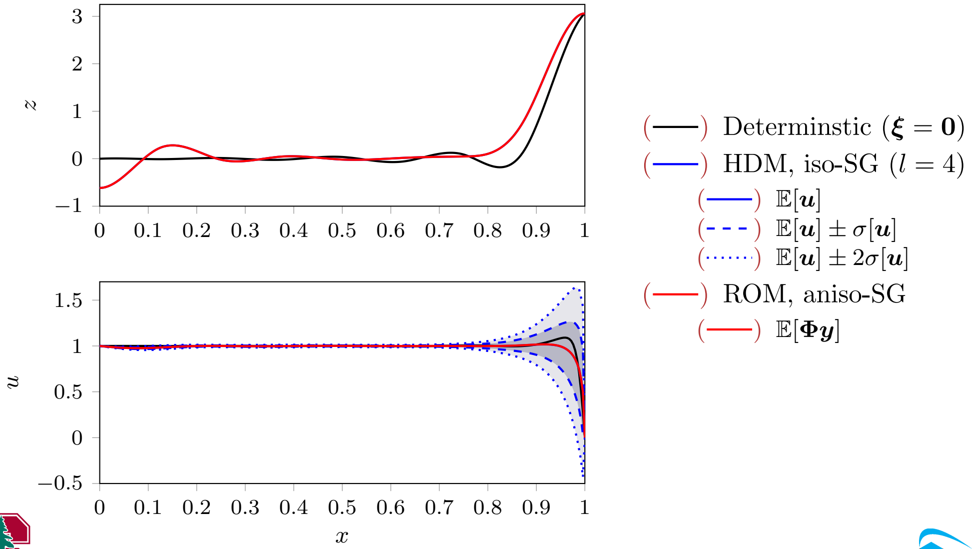

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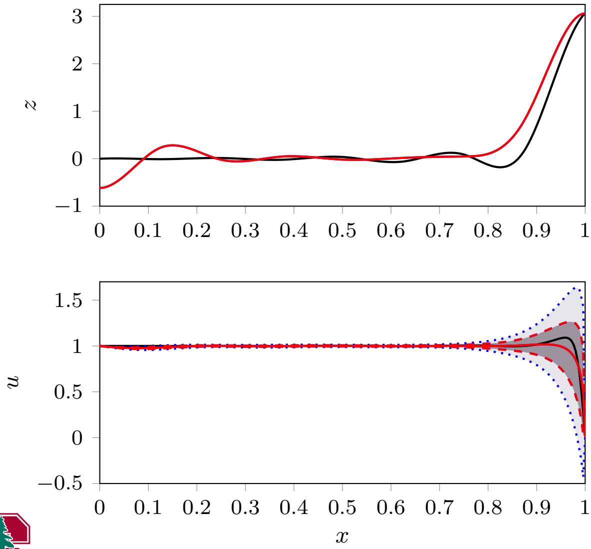

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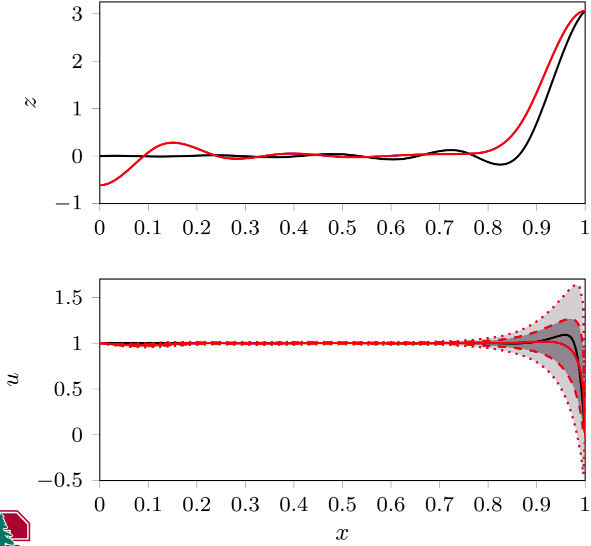
(——) HDM, iso-SG ($l = 4$)

- (——) $\mathbb{E}[\boldsymbol{u}]$
- (- - -) $\mathbb{E}[\boldsymbol{u}] \pm \sigma[\boldsymbol{u}]$
- (·······) $\mathbb{E}[\boldsymbol{u}] \pm 2\sigma[\boldsymbol{u}]$

(——) ROM, aniso-SG

- (——) $\mathbb{E}[\boldsymbol{\Phi y}]$
- (- - -) $\mathbb{E}[\boldsymbol{\Phi y}] \pm \sigma[\boldsymbol{\Phi y}]$

Trust-region method recovers optimal control and statistics



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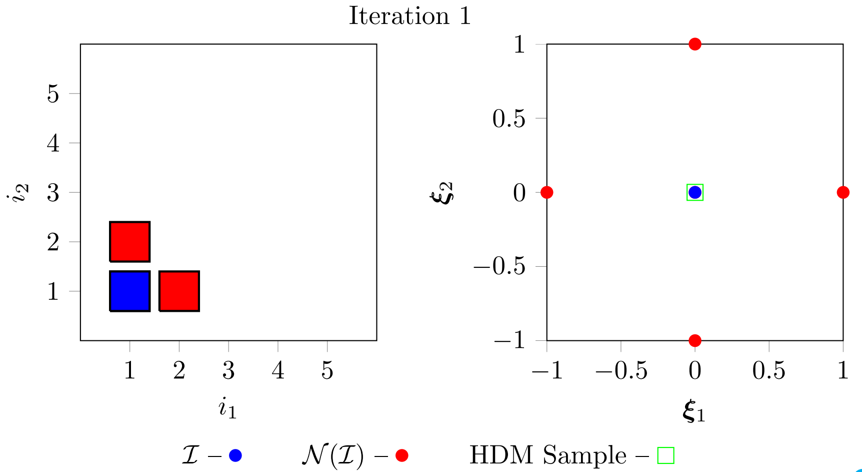
- ( ) $\mathbb{E}[\boldsymbol{u}] \pm \sigma[\boldsymbol{u}]$
- ( ) $\mathbb{E}[\boldsymbol{u}] \pm 2\sigma[\boldsymbol{u}]$

( ) ROM, aniso-SG

- ( ) $\mathbb{E}[\boldsymbol{\Phi y}]$
- ( ) $\mathbb{E}[\boldsymbol{\Phi y}] \pm \sigma[\boldsymbol{\Phi y}]$
- ( ) $\mathbb{E}[\boldsymbol{\Phi y}] \pm 2\sigma[\boldsymbol{\Phi y}]$

Trust-region method requires very few HDM queries to converge

Prior to each trust-region subproblem, the model (sparse grid, $\mathcal{I}_k$, and basis, $\mathbf{\Phi}_k$) must be constructed such that error indicators are below a tolerance



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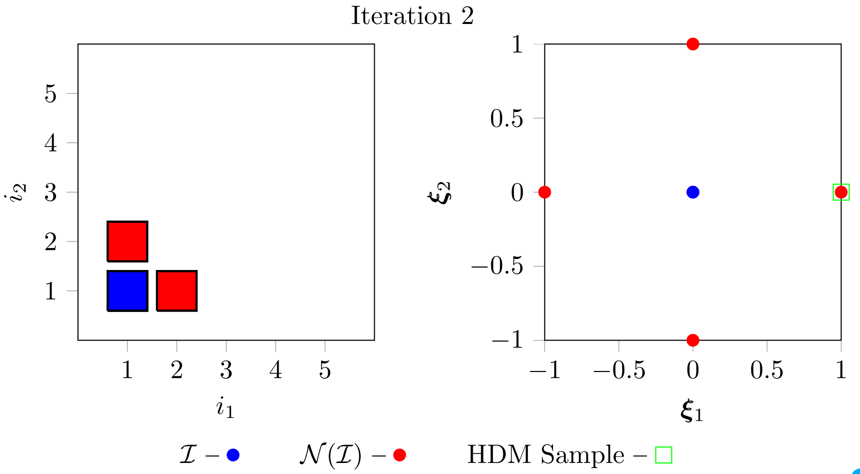

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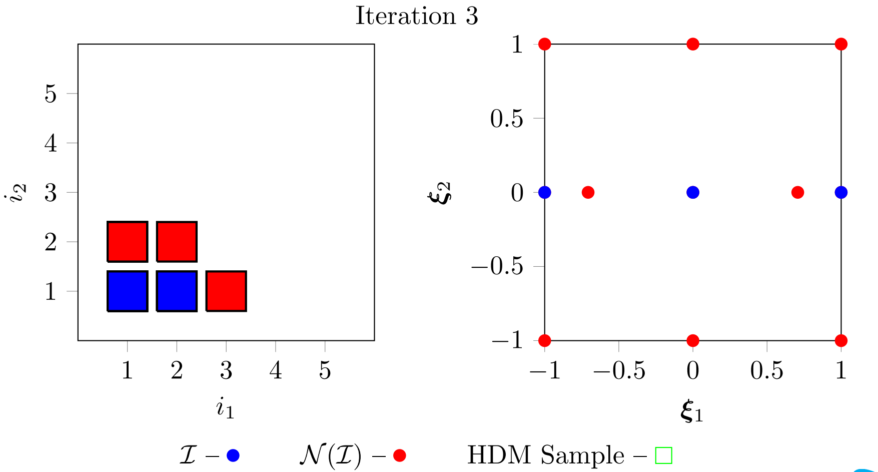

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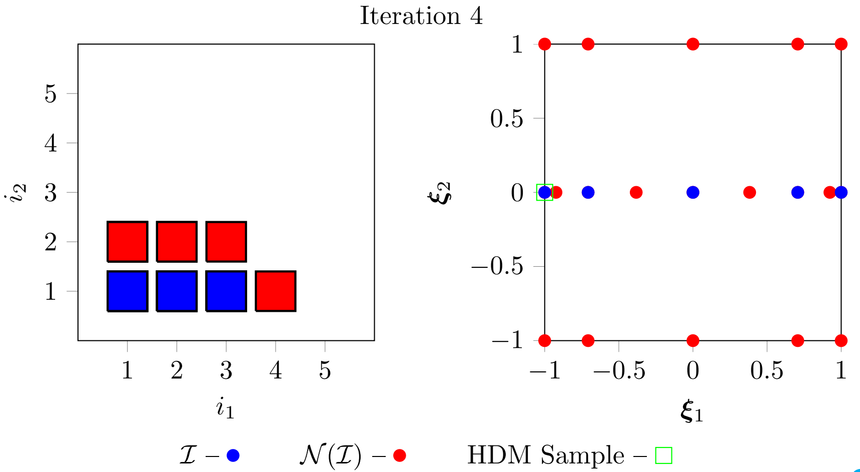

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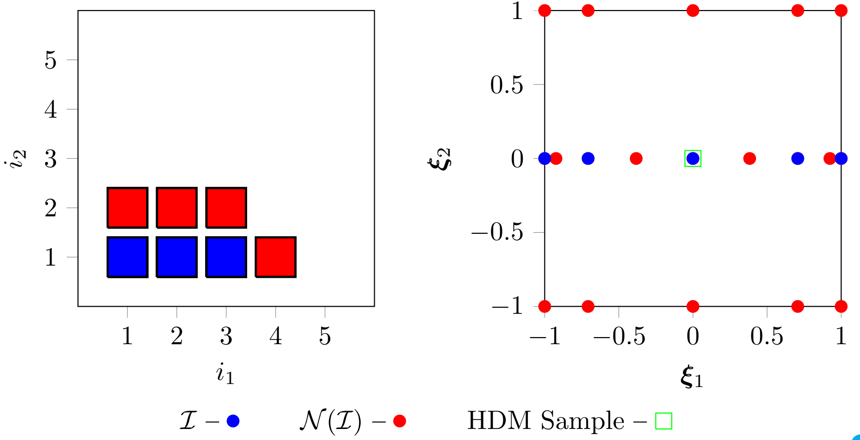
Iteration 5



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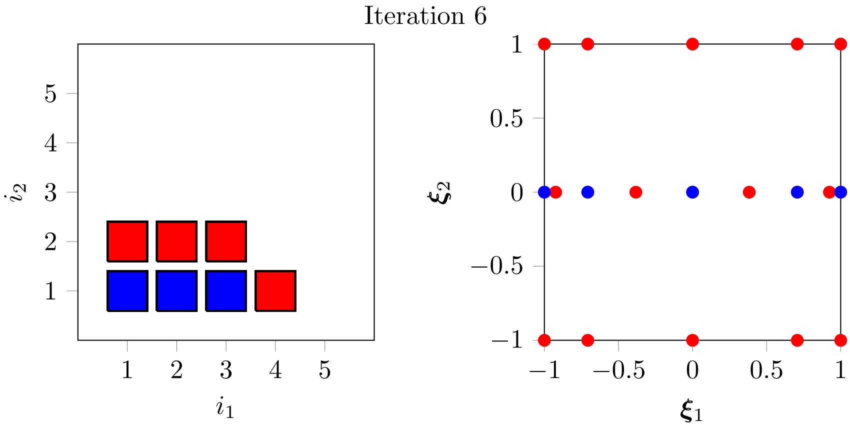
Prior to each trust-region subproblem, the model (sparse grid, $\mathcal{I}_k$, and basis, $\boldsymbol{\Phi}_k$) must be constructed such that error indicators are below a tolerance



$\mathcal{I}$ – ● $\mathcal{N}(\mathcal{I})$ – ● HDM Sample – □

Global convergence of trust-region method

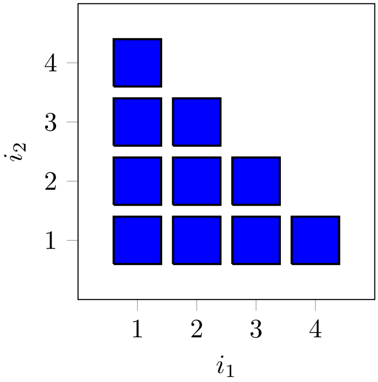
The trust-region method finds a sequence of parameters $\boldsymbol{\mu}_k$ *such that the gradient of HDM* $(||\nabla \mathcal{J}(\boldsymbol{\mu})||)$ *converges to* 0

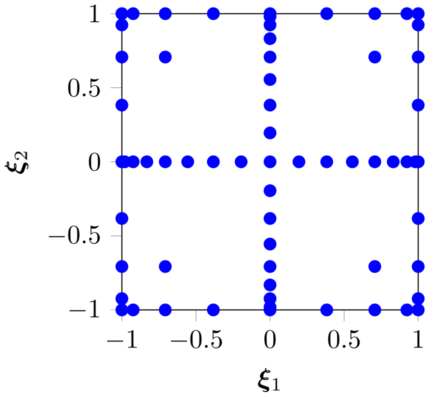
$m_k(\hat{\boldsymbol{\mu}}_k)$	$\|\|\nabla m_k(\hat{\boldsymbol{\mu}}_k)\|\|$	$\mathcal{J}(\hat{\boldsymbol{\mu}}_k)$	$\|\|\nabla \mathcal{J}(\hat{\boldsymbol{\mu}}_k)\|\|$	ρ_k	Δ_k	Success?
3.8783e-03	3.3779e-03	8.3351e-03	6.8542e-03	-	-	-
3.1121e-03	2.0393e-04	7.2687e-03	7.0676e-03	1.3918e+00	1.0000e+02	True
3.0474e-03	7.7900e-05	6.8352e-03	3.3518e-03	3.3943e-01	2.0000e+02	True
1.1910e-02	3.7019e-04	9.7269e-03	3.5655e-03	-2.6141e-01	1.0000e+02	False
6.3680e-03	9.6334e-06	6.3591e-03	8.6182e-05	1.0070e+00	2.8202e-03	True
6.3587e-03	7.2419e-07	6.3589e-03	7.2665e-07	1.0018e+00	5.6404e-03	True

Few HDM queries are required for convergence at the cost of many ROM queries

HDM Queries	ROM Queries (max size)
4	3720 (48)

1000× reduction in HDM queries vs. stochastic collocation on 4-level isotropic sparse grid





Iterations (L-BFGS)	HDM Queries	$\|\|\nabla \mathcal{J}\|\|$
34	6372	6.6064e-07

Leveraging and managing two-levels of inexactness for efficient stochastic PDE-constrained optimization

Summary

- *Trust-region method* with strong connection to model error indicators
- Two-level approximation of moments of quantities of interest of SPDE
  - *Anisotropic sparse grids* - inexact integration
  - *Reduced-order models* - inexact evaluations
- Two-level inexactness managed through trust-region method
- 1000$\times$ decrease in number of HDM queries

Future work

- Incorporate nonlinear constraints
- Local reduced-order models for improved efficiency
- Less expensive error indicators for cheaper trust-region subproblems [Drohmann and Carlberg, 2014]

References I

De Santis, D., Zahr, M. J., and Farhat, C. (January 4 - 8 (2016)).
Gradient-based aerodynamic shape optimization using the FIVER embedded boundary method.
In *AIAA Science and Technology Forum and Exposition (SciTech 2016)*, San Diego, California.

Drohmann, M. and Carlberg, K. (2014).
The romes method for statistical modeling of reduced-order-model error.
SIAM Journal on Uncertainty Quantification.

Gerstner, T. and Griebel, M. (2003).
Dimension–adaptive tensor–product quadrature.
Computing, 71(1):65–87.

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.

Zahr, M. J. and Farhat, C. (in preparation, 2016).
Roms for topology optimization.
International Journal for Numerical Methods in Engineering.

References II

Zahr, M. J. and Persson, P.-O. (In review, 2016).
An adjoint method for a high-order discretization of deforming domain conservation laws for optimization of flow problems.
Journal of Computational Physics.

Zahr, M. J., Persson, P.-O., and Wilkening, J. (In review, 2016).
A fully discrete adjoint method for optimization of flow problems on deforming domains with time-periodicity constraints.
Computers and Fluids.