Introduction to Reduced Basis Methods: Theory and Applications

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Remarks

My background

Goals

Limitations

Overview

Part I: Introduction to the Reduced Basis Method

Part II: The RB Method and Data

Part III: Applications

Exercises (by James Nichols)

Overview

Part I: Introduction to the Reduced Basis Method

Motivation

RB for the Simplest Case

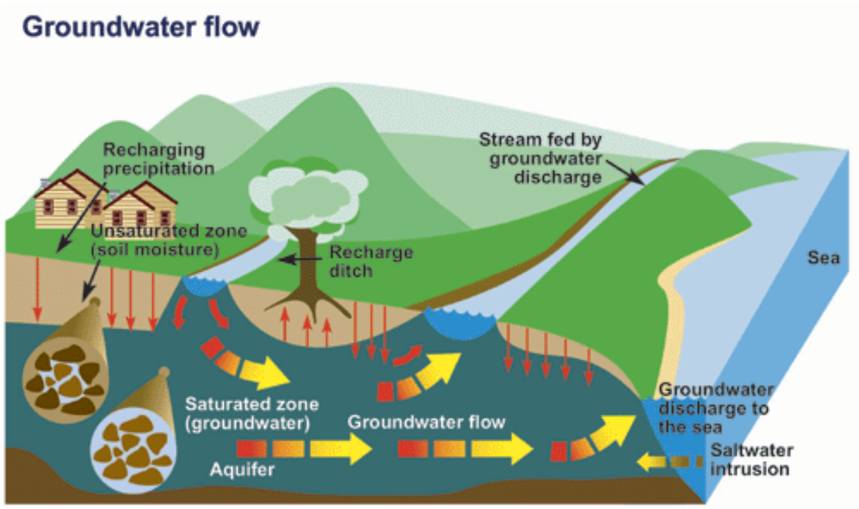
Generalizations

Part II: RB + Data

Part III: Applications + Exercises

PART I

Motivation - A Geosciences Example



Source: Environment and Climate Canada
`https://www.ec.gc.ca/eau-water`

Groundwater Flow:

- Groundwater management
- Contaminant transport

Goal:

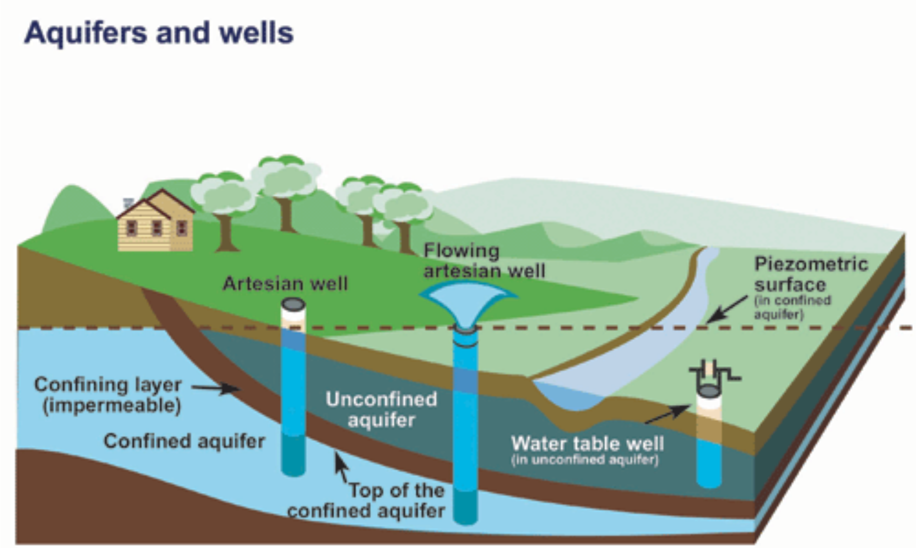
- Predict hydraulic head
- Predict pollutant concentration

Given:

- Parametrized PDE-model

Issues:

- Parameters unknown
- Model, but possibly erroneous
- Boundary or initial conditions uncertain
- Measurements, possibly noisy



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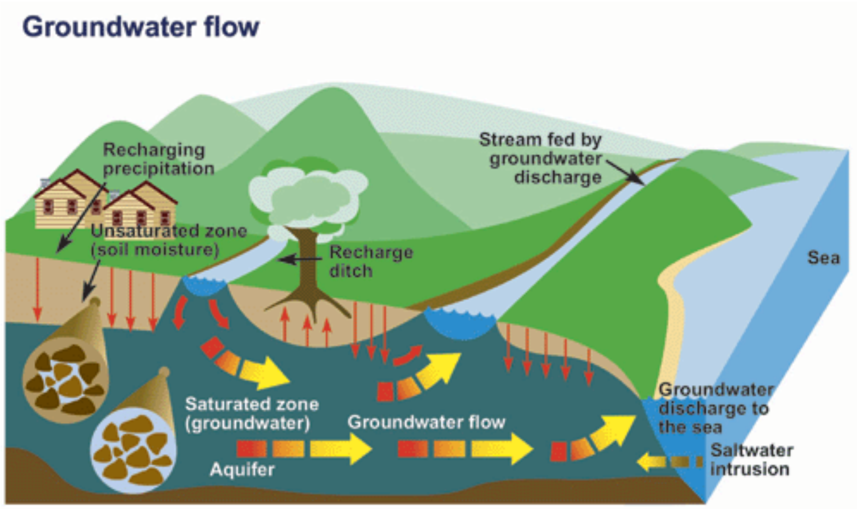
Motivation - A Geosciences Example



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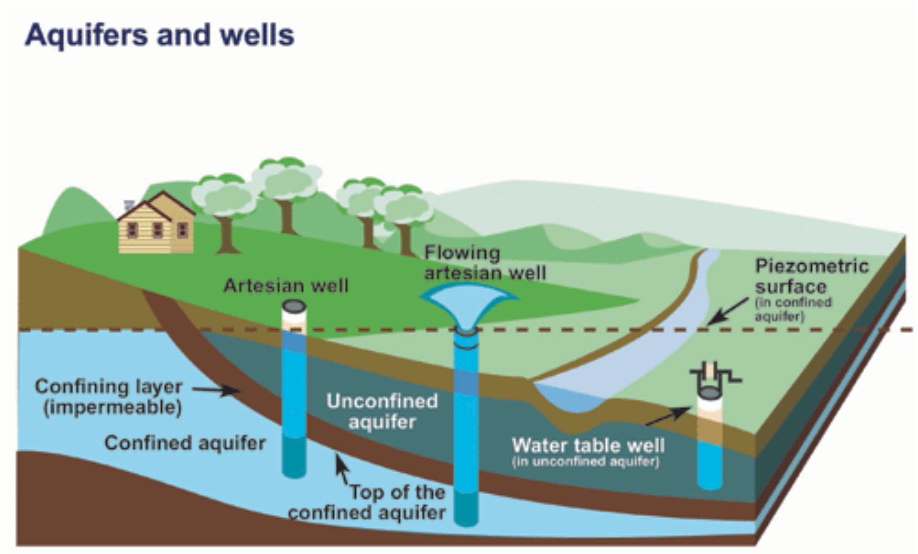

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Brief Introduction to the Reduced Basis Method

Notation

In the following:

μ	parameter
s	output
y	state, and $y(\mu) \equiv y(\boldsymbol{x}; \mu)$

Objective

Problem: Compute $s(\mu) = f(y(\mu); \mu)$ where

$$a(y(\mu), v; \mu) = f(v; \mu), \qquad \forall\, v \in \mathcal{Y} \qquad\qquad \text{PDE}$$

in multi-query, real-time, or slim computing settings.

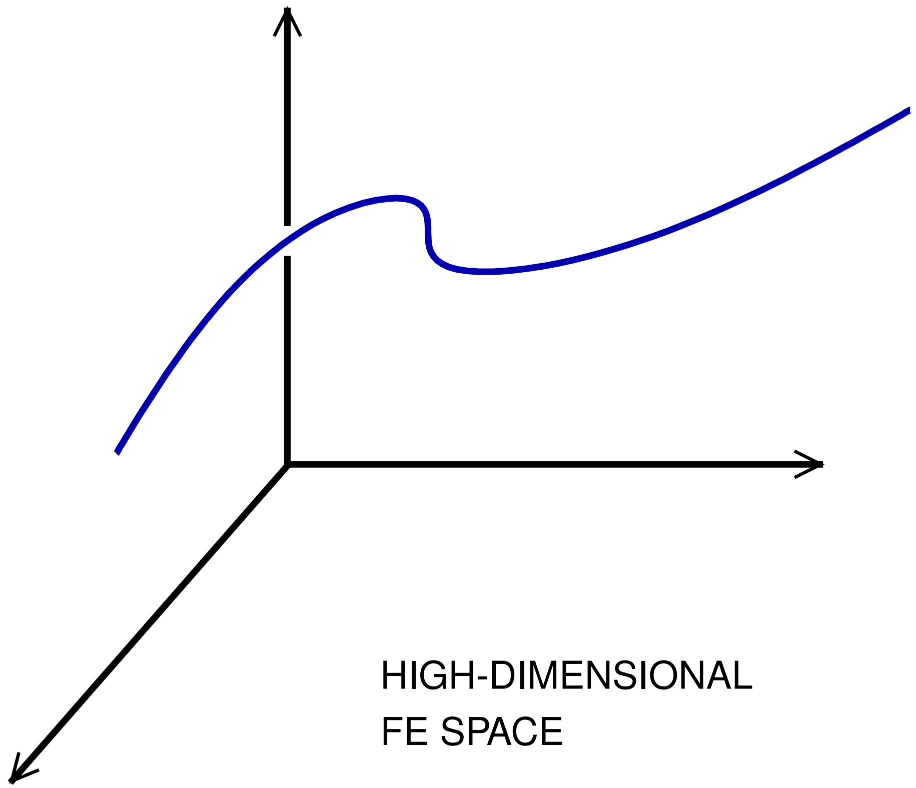
Goal: Compute approximations

$$y(\mu) \approx y_N(\mu)$$

$$s(\mu) \approx s_N(\mu) := f(y_N(\mu); \mu)$$

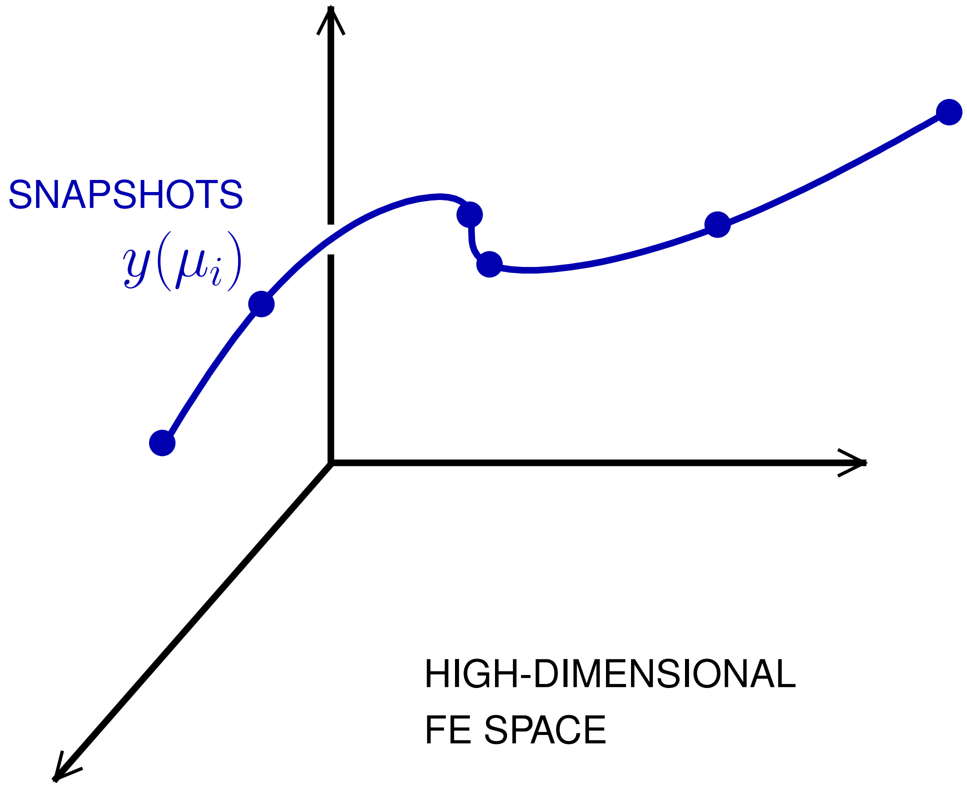
that are (certifiably-)accurate and (online-)inexpensive.

The Reduced Basis Method



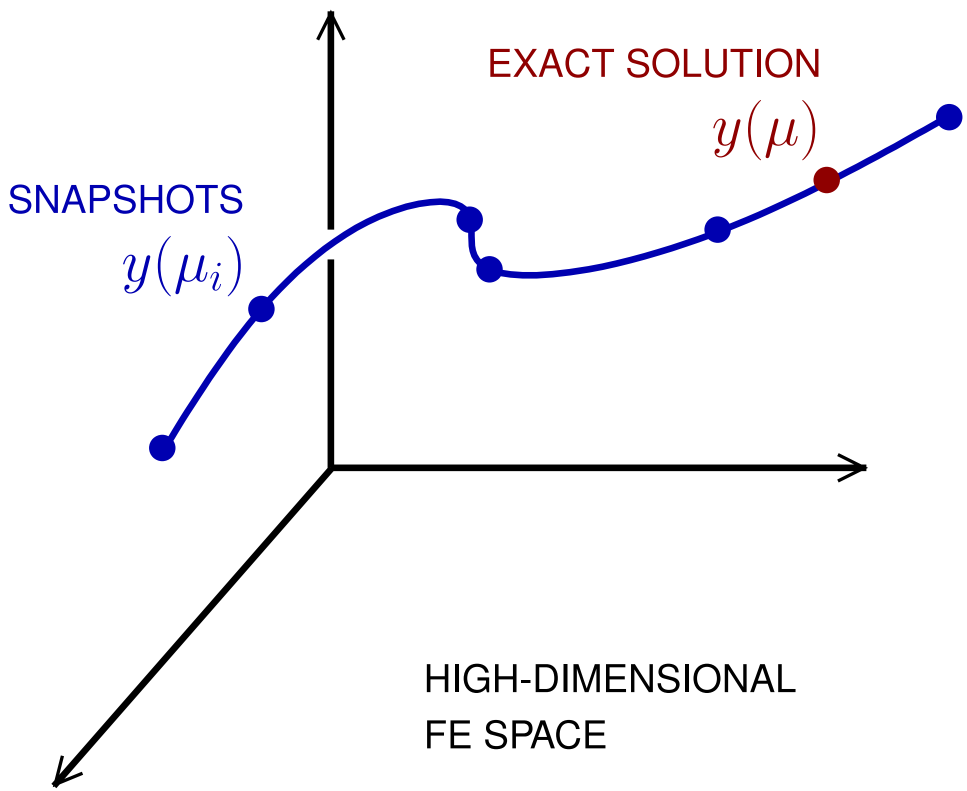
$$a(y(\mu), v; \mu) = f(v; \mu), \quad \text{for all } v \in \mathcal{Y}$$

The Reduced Basis Method



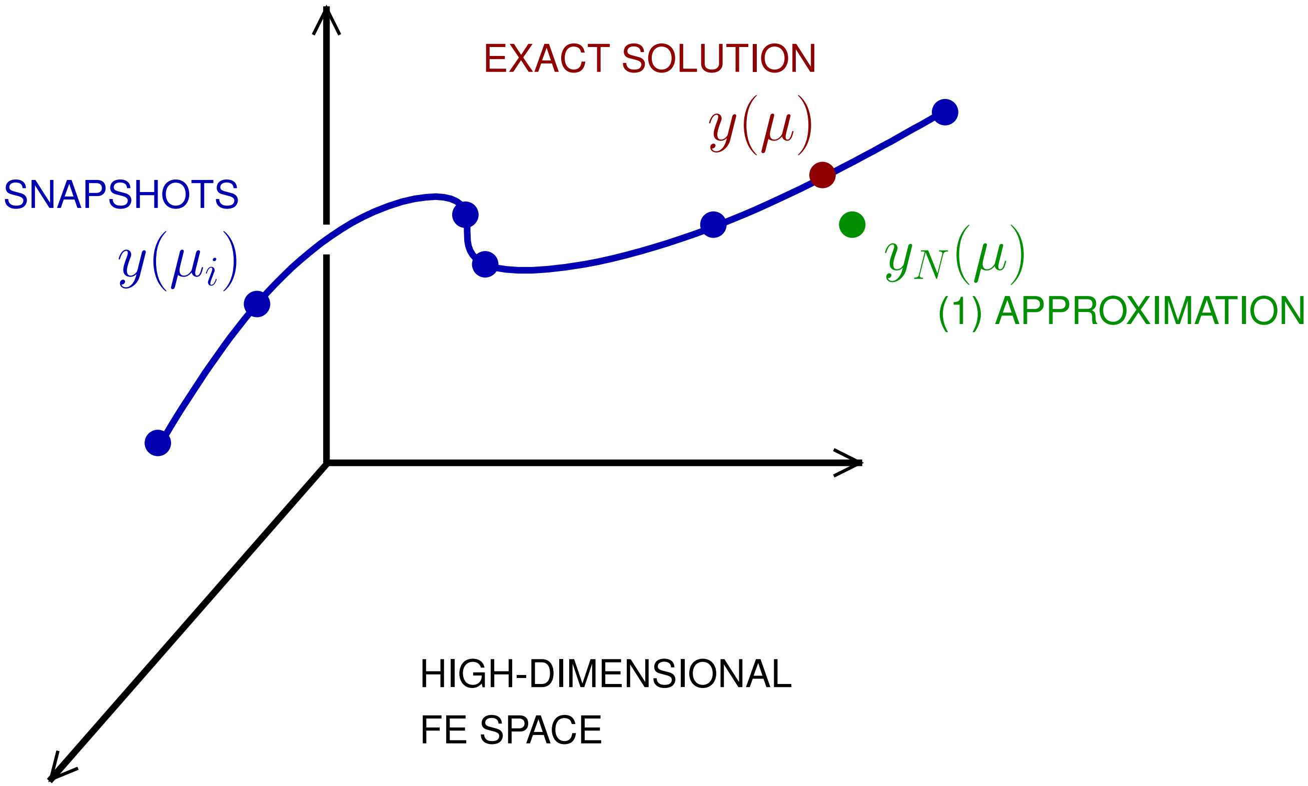
$$\mathcal{Y}_N = \text{span}\{\ y(\mu_i)\,,\ i = 1, \ldots, N\ \}$$

The Reduced Basis Method



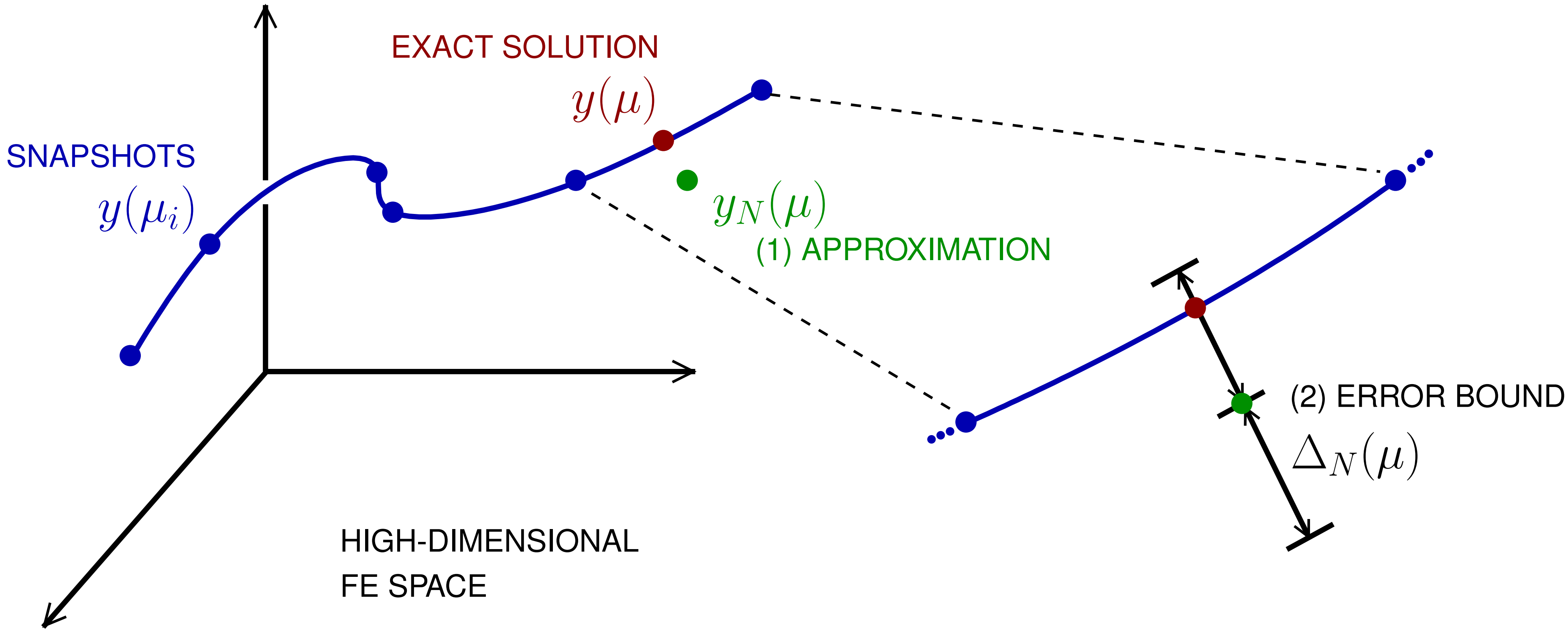
$$a(y(\mu), v; \mu) = f(v; \mu), \quad \text{for all } v \in \mathcal{Y}.$$

The Reduced Basis Method



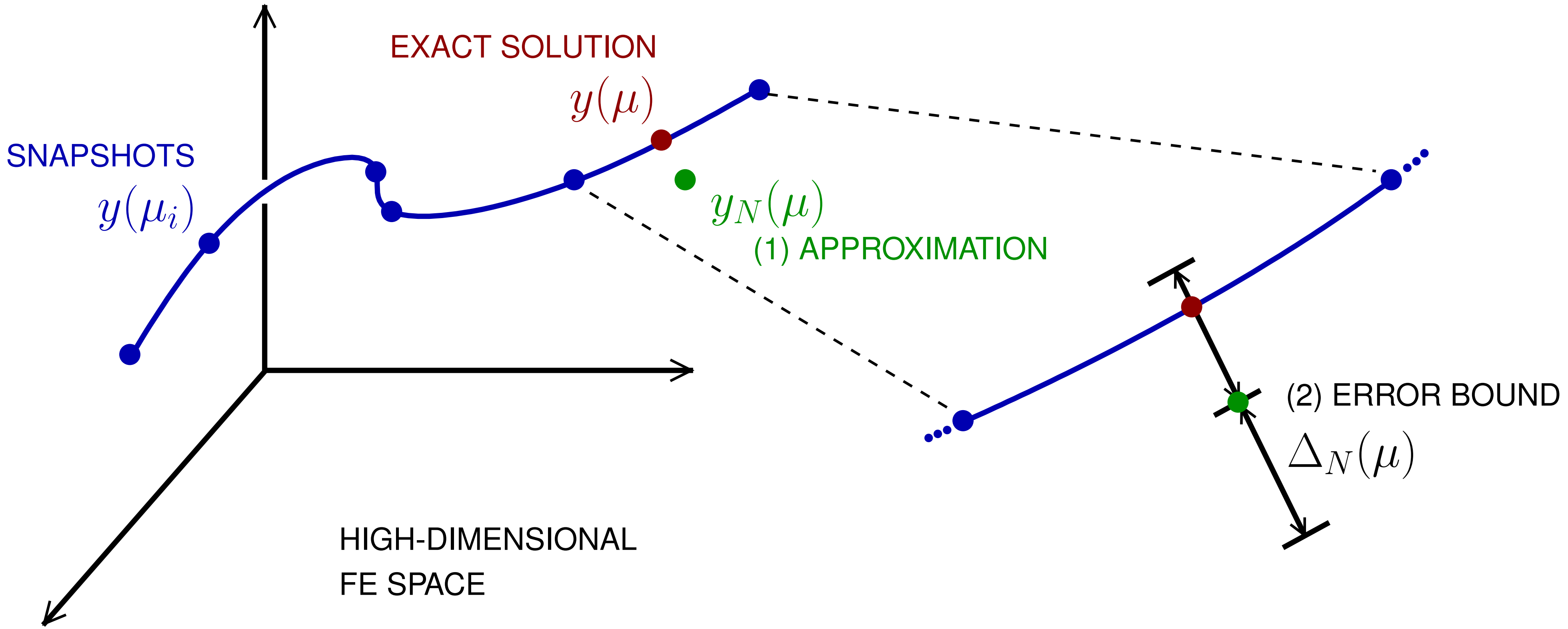
$$a(y_N(\mu), v; \mu) = f(v; \mu), \quad \text{for all } v \in \mathcal{Y}_N.$$

The Reduced Basis Method



$$\|y(\mu) - y_N(\mu)\|_{\mathcal{Y}} \;\leq\; \Delta_N(\mu).$$

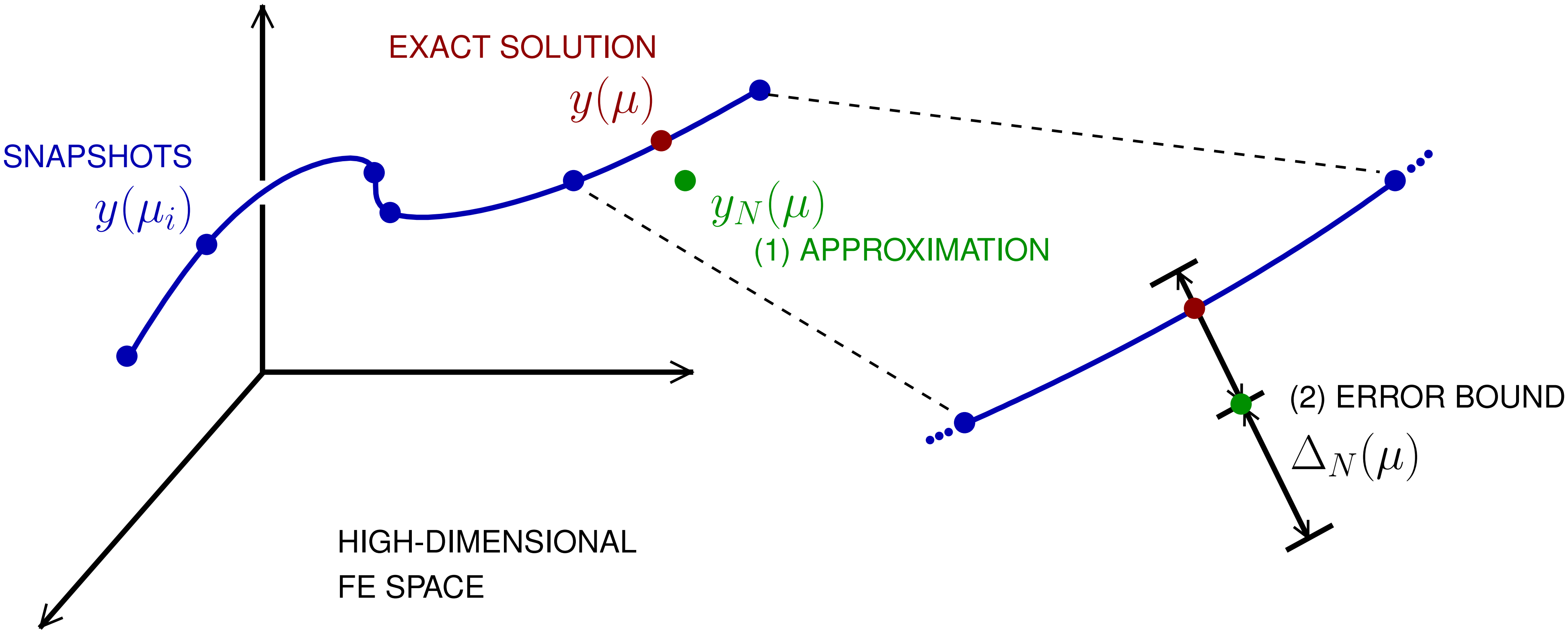
The Reduced Basis Method



(3) OFFLINE-ONLINE COMPUTATIONAL DECOMPOSITION

$$a(w,v;\mu) = \sum_{q=1}^{Q} \underbrace{\theta^q(\mu)}_{\mu\text{- DEPENDENT COEFFICIENTS}} \underbrace{a^q(w,v)}_{\mu\text{- INDEPENDENT BILINEAR FORMS}}, \quad \forall w,v \in \mathcal{Y}$$

The Reduced Basis Method

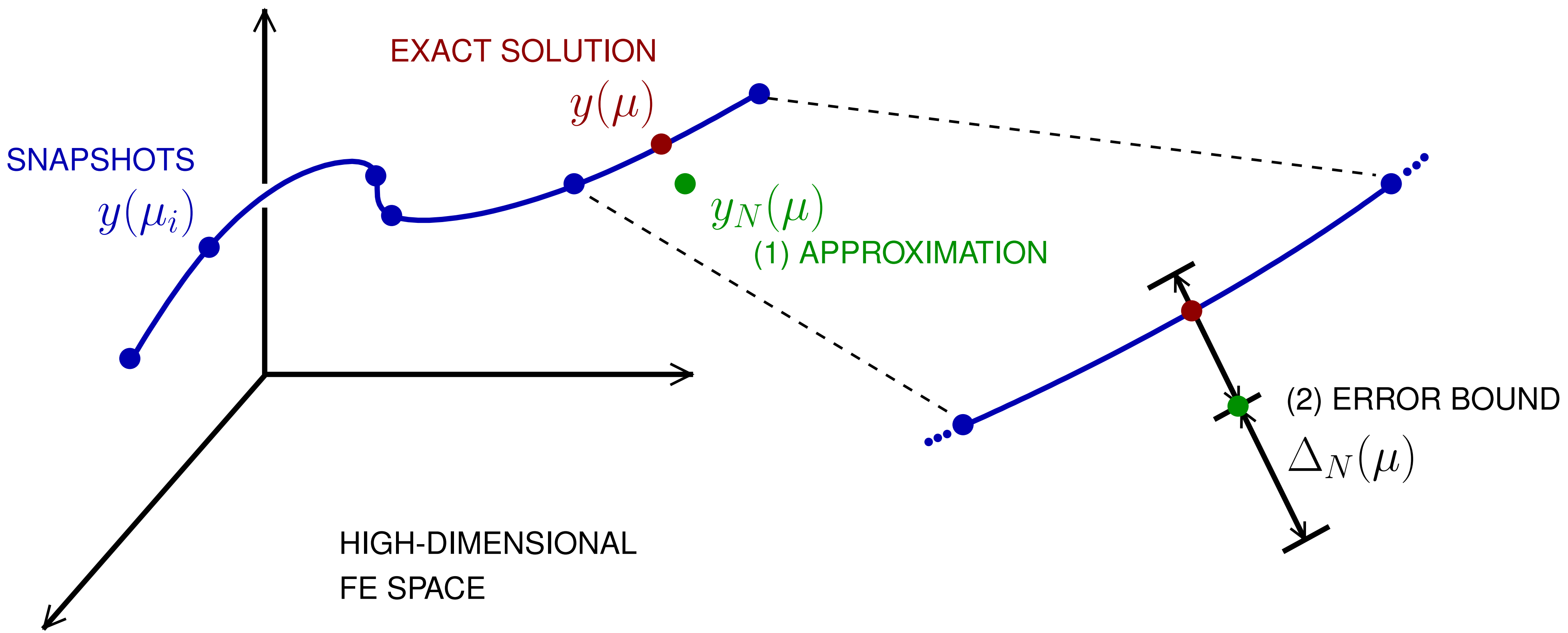


(3) OFFLINE-ONLINE COMPUTATIONAL DECOMPOSITION

(4) GREEDY ALGORITHM

$$\mu_{N+1} = \arg\max_{\mu \in \mathcal{D}} \frac{\Delta_N(\mu)}{\|y_N(\mu)\|_{\mathcal{Y}}}$$

The Reduced Basis Method



(3) OFFLINE-ONLINE COMPUTATIONAL DECOMPOSITION
(4) GREEDY ALGORITHM

The Reduced Basis Method

The **reduced basis method** seeks to provide, for any $\mu \in \mathcal{D}$

accurate	$y_N(\mu) \approx y(\mu)$	**(1) APPROX**
reliable	$\|y(\mu) - y_N(\mu)\|_{\mathcal{Y}} \geq \Delta_N(\mu)$	**(2) ERR ES**
efficient surrogates	cost $(Q^\bullet, N^\bullet)$	**(3) DECOMP**
	small N	**(4) GREEDY**

to solutions of **parametrized PDEs**

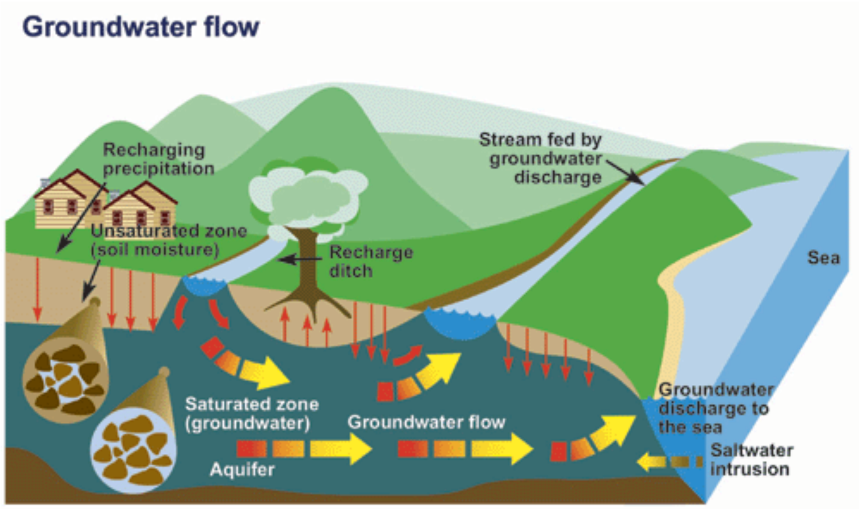
for the **many-query**, **real-time**,

and **slim-computing** contexts.

[Prud'homme, et al., 2002], [Maday, et al., 2002], …

[Hesthaven, Rozza & Stamm, 2015], [Quarteroni, Manzoni & Negri, 2015]

Motivation - A Geosciences Example



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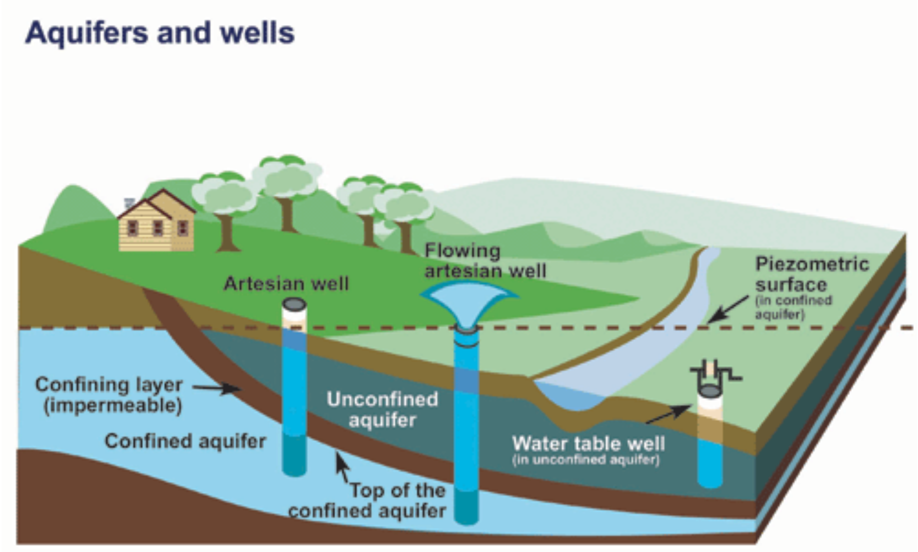

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Simplest Case: Poisson Problem

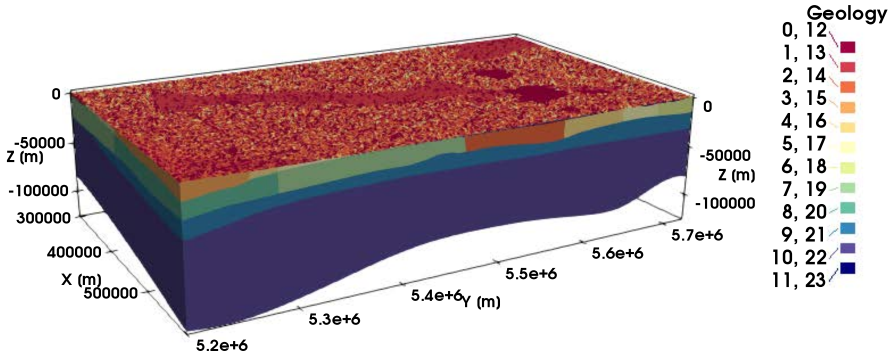
Strong Form

Find y such that

$$\text{PDE} \quad -\kappa\nabla^2 y = f \quad \text{in} \quad \Omega \subset \mathbb{R}^3 \qquad \text{domain}$$

$$\text{BC} \quad y = 0 \quad \text{on} \quad \Gamma_N \qquad \text{boundary}$$

where $\kappa = \begin{cases} 1 & \text{in} \quad \Omega_o \\ \kappa_i & \text{in} \quad \Omega_i,\ i = 1 \ldots P \end{cases}$



Upper Rhine Graben (Germany)

Courtesy of Prof. Scheck-Wenderoth, GFZ Postdam.

Let $\quad \mu = \{\kappa_1, \ldots, \kappa_P\} \in \mathcal{D} \subset \mathbb{R}^P$ $\qquad$ parameter

Simplest Case: Poisson Problem

Weak Form

Find $y \equiv y(\mu) \in \mathcal{Y}$ s.t.

$$\kappa_o \sum_{i=0}^{p} \int_{\Omega_i} \nabla y \cdot \nabla v \, d\Omega \;=\; \int_{\Omega} v \, d\Omega, \quad \forall\, v \in \mathcal{Y},$$

and compute $s(\mu) = \int_{\Omega} y(\mu)\, d\Omega\,.$

Abstract Form

Find $y = y(\mu) \in \mathcal{Y}$ s.t.

$$a(y(\mu), v; \mu) \;=\; f(v; \mu), \quad \forall\, v \in \mathcal{Y},$$

and compute $s(\mu) \;=\; f(y(\mu); \mu).$

Simplest Case: Poisson Problem

General Form

Find $y(\mu) \in \mathcal{Y}$ s.t.

$$a(y(\mu), v; \mu) \;=\; f(v; \mu)$$

$$\forall\, v \in \mathcal{Y}$$

Matrix Form

Find $\boldsymbol{y}_{\mathcal{N}}(\mu) \in \mathbb{R}^{\mathcal{N}}$ s.t.

$$\boldsymbol{A}_{\mathcal{N}}(\mu)\boldsymbol{y}_{\mathcal{N}}(\mu) \;=\; \boldsymbol{f}_{\mathcal{N}}(\mu),$$

where $\boldsymbol{A}_{\mathcal{N}} \in \mathbb{R}^{\mathcal{N}\times\mathcal{N}},\ \boldsymbol{f}_{\mathcal{N}} \in \mathbb{R}^{\mathcal{N}}$

Questions:

How can we compute an approximation $y_N(\mu)$ to $y(\mu)$?

How do we know the error is small?

How do we know what value of N to take?

How do we compute $y_N(\mu),\ s_N(\mu)$ efficiently online?

How do we choose the sample points μ_i optimally?

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Let $y_N(\mu) \in \mathcal{Y}_N \;:=\; \mathrm{span}\{\underbrace{y(\mu_1),\ldots,y(\mu_N)}_{\text{snapshots}}\} \;=\; \mathrm{span}\{\underbrace{\varphi_1,\ldots,\varphi_N}_{\text{orthogonal basis}}\}$

$$y_N(\mu) \;=\; \sum_{i=1}^{N} (\mathbf{y}_N)_i\, \varphi_i$$

Find $y_N(\mu) \in \mathcal{Y}_N$ s.t.

$$a(y_N(\mu), v; \mu) \;=\; f(v;\mu), \qquad \forall\, v \in \mathcal{Y}_N$$

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Simplest Case: Poisson Problem

Problem: Find $\boldsymbol{y}_{\mathcal{N}}(\mu) \in \mathbb{R}^{\mathcal{N}}$ s.t. $\boldsymbol{v}_{\mathcal{N}}^T \boldsymbol{\mathcal{A}}_{\mathcal{N}}(\mu) \boldsymbol{y}_{\mathcal{N}}(\mu) = \boldsymbol{v}_{\mathcal{N}}^T \boldsymbol{f}_{\mathcal{N}}(\mu), \ \forall\, \boldsymbol{v}_{\mathcal{N}} \in \mathbb{R}^{\mathcal{N}}$

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Let $\boldsymbol{y}_N(\mu) \in \mathrm{span}\{ \boldsymbol{\varphi}_i, \ldots, \boldsymbol{\varphi}_N \}$, and $\boldsymbol{\mathcal{W}}_N = [\, \boldsymbol{\varphi}_i, \ldots, \boldsymbol{\varphi}_N \,]$

$$\underbrace{\boldsymbol{y}_N(\mu)}_{\substack{\text{approximation} \\ \text{to } \boldsymbol{y}_{\mathcal{N}}(\mu)}} = \sum_{i=1}^{N} \underbrace{(\mathbf{y}_N)_i(\mu)}_{\text{coefficients}} \underbrace{\boldsymbol{\varphi}_i}_{\text{snapshots}} = \boldsymbol{\mathcal{W}}_N \mathbf{y}_N \,.$$

Similarly, let $\boldsymbol{v}_N = \boldsymbol{\mathcal{W}}_N \, \mathrm{v}_N$

Simplest Case: Poisson Problem

Problem: Find $\boldsymbol{y}_{\mathcal{N}}(\mu) \in \mathbb{R}^{\mathcal{N}}$ s.t. $\boldsymbol{v}_{\mathcal{N}}^T \boldsymbol{A}_{\mathcal{N}}(\mu)\boldsymbol{y}_{\mathcal{N}}(\mu) = \boldsymbol{v}_{\mathcal{N}}^T \boldsymbol{f}_{\mathcal{N}}(\mu), \; \forall\, \boldsymbol{v}_{\mathcal{N}} \in \mathbb{R}^{\mathcal{N}}$

Let $\boldsymbol{y}_N(\mu) \in \mathrm{span}\{\, \boldsymbol{\varphi}_i, \ldots, \boldsymbol{\varphi}_N \,\}$, and $\boldsymbol{\mathcal{W}}_N = [\, \boldsymbol{\varphi}_i, \ldots, \boldsymbol{\varphi}_N \,]$

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Similarly, let $\boldsymbol{v}_N = \boldsymbol{\mathcal{W}}_N \, \mathrm{v}_N$

Find $\boldsymbol{y}_N(\mu) \in \mathrm{colsp}\, \boldsymbol{\mathcal{W}}_N$ s.t.

$$\boldsymbol{v}_N^T \boldsymbol{\mathcal{A}}(\mu)\, \boldsymbol{y}_N(\mu) = \boldsymbol{v}_N^T \boldsymbol{f}(\mu), \quad \forall\, \boldsymbol{v}_N \in \mathrm{colsp}\, \boldsymbol{\mathcal{W}}_N$$

$$\Rightarrow \quad \mathbf{v}_N^T \boldsymbol{\mathcal{W}}_N^T \boldsymbol{\mathcal{A}}(\mu)\, \boldsymbol{\mathcal{W}}_N \,\mathbf{y}_N(\mu) = \mathbf{v}_N^T \boldsymbol{\mathcal{W}}_N^T \boldsymbol{f}(\mu), \quad \forall\, \mathbf{v}_N \in \mathbb{R}^{\mathcal{N}}$$

Simplest Case: Poisson Problem

$$\mathbf{v}_N^T \underbrace{\mathcal{W}_N^T \, \mathcal{A}(\mu) \, \mathcal{W}_N}_{\mathbf{A}_N(\mu)} \, \mathbf{y}_N(\mu) = \mathbf{v}_N^T \underbrace{\mathcal{W}_N^T \, \boldsymbol{f}(\mu)}_{\mathbf{f}_N(\mu)} \quad \forall \, \mathbf{v}_N \in \mathbb{R}^{\mathrm{N}}$$

$$\Rightarrow \quad \mathbf{v}_N^T \, \mathbf{A}_N(\mu) \, \mathbf{y}_N(\mu) = \mathbf{v}_N^T \mathbf{f}_N(\mu), \qquad \forall \, \mathbf{v}_N \in \mathbb{R}^{\mathrm{N}}$$

$$\Rightarrow \quad \mathbf{A}_N(\mu) \, \mathbf{y}_N(\mu) = \mathbf{f}_N(\mu)$$

coefficients in expansion
in terms of the basis

Simplest Case: Poisson Problem

General Form

Find $y_N(\mu) \in \mathcal{Y}_N$ s.t.

$$a(y_N(\mu), v; \mu) = f(v; \mu) \quad \forall\, v \in \mathcal{Y}_N$$

Matrix Form

Find $\mathbf{y}_N(\mu) \in \mathbb{R}^N$ s.t.

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Simplest Case: Poisson Problem

Problem: Find $y(\mu) \in \mathcal{Y}$ s.t. $a(y(\mu), v; \mu) \;=\; f(v;\mu), \quad \forall\, v \in \mathcal{Y}$

(Lax-Milgram) Let $\mathcal{Y}$ be a Hilbert space, and for all $\mu \in \mathcal{D}$, assume

- $a(\cdot,\cdot;\mu)$ is continuous and coercive,

$$\gamma_a(\mu) \;:=\; \sup_{u\in\mathcal{Y}} \sup_{w\in\mathcal{Y}} \frac{a(v,w;\mu)}{\|v\|_{\mathcal{Y}}\|w\|_{\mathcal{Y}}} < \infty$$

$$\alpha_a(\mu) := \inf_{v\in\mathcal{Y}} \frac{a(v,v;\mu)}{\|v\|^2_{\mathcal{Y}}} > 0$$

- f is bounded,

$$\|f\|_{\mathcal{Y}'} := \sup_{v\in\mathcal{Y}} \frac{f(v)}{\|v\|_{\mathcal{Y}}} < \infty.$$

Then there exists a unique solution $y(\mu)$ satisfying

$$\|y(\mu)\|_{\mathcal{Y}} \leq \frac{\|f\|_{\mathcal{Y}'}}{\alpha_a(\mu)}.$$

Simplest Case: Poisson Problem

Consider the following

$$a(y(\mu), v; \mu) \;=\; f(v; \mu), \quad \forall\, v \in \mathcal{Y}, \qquad \text{FE problem}$$

$$a(y_N(\mu), v; \mu) \;=\; f(v; \mu), \quad \forall\, v \in \mathcal{Y}_N. \qquad \text{RB approximation}$$

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Consider the following

$$a(y(\mu), v; \mu) = f(v; \mu), \quad \forall\, v \in \mathcal{Y}, \qquad \text{FE problem}$$

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Define the error $e_N(\mu) := y(\mu) - y_N(\mu)$ and the residual

$$\begin{aligned} r(v; y_N(\mu); \mu) &:= f(v; \mu) - a(y_N(\mu), v; \mu), \quad \text{for } v \in \mathcal{Y} \\ &= a(y(\mu), v; \mu) - a(y_N(\mu), v; \mu) \\ &= a(y(\mu) - y_N(\mu), v; \mu) \\ &= a(e_N(\mu), v; \mu) \end{aligned}$$

Simplest Case: Poisson Problem

From the error-residual equation

$$a(e_N(\mu), v; \mu) \;=\; r(v; y_N(\mu), \mu)$$

Simplest Case: Poisson Problem

From the error-residual equation

$$a(e_N(\mu), v; \mu) \;=\; r(v; y_N(\mu), \mu)$$

and the Lax-Milgram Theorem, we have that

$$\|e_N(\mu)\|_{\mathcal{Y}} \;\leq\; \frac{\|r(\cdot; y_N(\mu), \mu)\|_{\mathcal{Y}'}}{\alpha_a(\mu)}.$$

Simplest Case: Poisson Problem

From the error-residual equation

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and the Lax-Milgram Theorem, we have that

$$\|e_N(\mu)\|_{\mathcal{Y}} \;\leq\; \frac{\|r(\cdot; y_N(\mu), \mu)\|_{\mathcal{Y}'}}{\alpha_a(\mu)}.$$

Assume we have a computable lower bound $\alpha_a^{\mathrm{LB}}(\mu) \leq \alpha_a(\mu), \; \forall\, \mu \in \mathcal{D}$.

Then $$\|e_N(\mu)\|_{\mathcal{Y}} \;\leq\; \Delta_N(\mu) \;:=\; \frac{\|r(\cdot; y_N(\mu))\|_{\mathcal{Y}'}}{\alpha_a^{\mathrm{LB}}(\mu)}$$ ERR BOUND

Simplest Case: Poisson Problem

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Find $y_N(\mu) \in \mathcal{Y}_N$ s.t.

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Matrix Form

Find $\mathbf{y}_N(\mu) \in \mathbb{R}^N$ s.t.

$$\mathbf{A}_N(\mu)\mathbf{y}_N(\mu) \; = \; \mathbf{f}_N(\mu),$$

where $\mathbf{A}_N \in \mathbb{R}^{N\times N}$, $\mathbf{f}_N \in \mathbb{R}^N$

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Simplest Case: Poisson Problem

Problem: How can we compute $\mathbf{y}_N(\mu)$ efficiently?

We have $\mathbf{A}_N(\mu)\,\mathbf{y}_N(\mu) = \mathbf{f}_N(\mu)$ where

$$\mathbf{A}_N(\mu) = \boldsymbol{\mathcal{W}}_N^T \boldsymbol{\mathcal{A}}_{\mathcal{N}}(\mu)\, \boldsymbol{\mathcal{W}}_N \text{ and } \mathbf{f}_N(\mu) = \boldsymbol{\mathcal{W}}_N^T \boldsymbol{f}_{\mathcal{N}}(\mu)$$

Assume that $\boldsymbol{\mathcal{A}}_{\mathcal{N}}(\mu)$ and $\boldsymbol{f}_{\mathcal{N}}(\mu)$ are affine in the parameter, i.e.

$$\boldsymbol{\mathcal{A}}_{\mathcal{N}}(\mu) = \sum_{q=1}^{Q_a} \underbrace{\theta_a^q(\mu)}_{\mu\text{-dependent coefficients}} \underbrace{\boldsymbol{\mathcal{A}}_{\mathcal{N}}^q}_{\mu\text{-independent matrices}} \text{ and } \boldsymbol{f}_{\mathcal{N}}(\mu) = \sum_{q=1}^{Q_f} \theta_f^q(\mu)\; \boldsymbol{f}_{\mathcal{N}}^q .$$

For our Poisson example

$$\underbrace{a(w,v;\mu)}_{} = \sum_{q=0}^{P} \underbrace{\kappa_q}_{} \underbrace{\int_{\Omega_q} \nabla w \cdot \nabla v \, d\Omega}_{}$$

$$\boldsymbol{v}_{\mathcal{N}}^T \boldsymbol{\mathcal{A}}_{\mathcal{N}}(\mu)\, \boldsymbol{w}_{\mathcal{N}} = \sum_{q=0}^{P} \theta^q(\mu) \quad \boldsymbol{v}_{\mathcal{N}}^T \boldsymbol{\mathcal{A}}_{\mathcal{N}}^q\, \boldsymbol{w}_{\mathcal{N}}$$

Simplest Case: Poisson Problem

We thus obtain:

$$\mathbf{A}_N(\mu) = \boldsymbol{\mathcal{W}}_N^T \left(\sum_{q=1}^{\theta_a} \theta_a^q(\mu)\, \boldsymbol{\mathcal{A}}_{\mathcal{N}}^q \right) \boldsymbol{\mathcal{W}}_N = \sum_{q=1}^{Q_a} \theta_a^q(\mu) \Big(\underbrace{\boldsymbol{\mathcal{W}}_N^T \boldsymbol{\mathcal{A}}_{\mathcal{N}}^q \boldsymbol{\mathcal{W}}_N}_{\substack{\mu\text{-independent} \\ \text{matrices of size } N \times N}} \Big) = \sum_{q=1}^{Q_a} \theta_a^q(\mu)\, \mathbf{A}_N^q$$

Similarly, $\mathbf{f}_N(\mu) = \sum_{q=1}^{Q} \theta_f^q(\mu)\, (\boldsymbol{\mathcal{W}}_N^T \boldsymbol{f}_{\mathcal{N}}^q) = \sum_{q=1}^{Q} \theta_f^q\,(\mu) \mathbf{f}_N^q$

Simplest Case: Poisson Problem

We thus obtain:

$$\mathbf{A}_N(\mu) = \mathcal{W}_N^T \left(\sum_{q=1}^{\theta_a} \theta_a^q(\mu)\, \mathcal{A}_\mathcal{N}^q \right) \mathcal{W}_N = \sum_{q=1}^{Q_a} \theta_a^q(\mu) \Big(\underbrace{\mathcal{W}_N^T \mathcal{A}_\mathcal{N}^q\, \mathcal{W}_N}_{\substack{\mu\text{-independent} \\ \text{matrices of size } N \times N}} \Big) = \sum_{q=1}^{Q_a} \theta_a^q(\mu)\, \mathbf{A}_N^q$$

Similarly, $\mathbf{f}_N(\mu) = \sum_{q=1}^{Q} \theta_f^q(\mu)\, (\mathcal{W}_N^T \boldsymbol{f}_\mathcal{N}^q) = \sum_{q=1}^{Q} \theta_f^q\,(\mu) \mathbf{f}_N^q$

Offline stage:

- compute snapshot-basis $\mathcal{W}_N$
- compute and store $\mathbf{A}_N^q,\ \mathbf{f}_N^q$ at cost $(\mathcal{N}^\bullet, N^\bullet)$

Online stage:

For any $\mu \in \mathcal{D}$

- assemble $\mathbf{A}_N(\mu),\ \mathbf{f}_N(\mu)$
- solve for $\mathbf{y}_N(\mu)$ at cost $(N^\bullet)$

Simplest Case: Poisson Problem

How can we compute $\Delta_N(\mu)$ efficiently?

$$\Delta_N(\mu) = \frac{\|r(\cdot; y_N(\mu), \mu)\|_{\mathcal{Y}'}}{\alpha_a^{\mathrm{LB}}(\mu)}$$

where we assume we have $\alpha_a^{\mathrm{LB}}(\mu)$. SCM

Simplest Case: Poisson Problem

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where we assume we have $\alpha_a^{\mathrm{LB}}(\mu)$. SCM

Let $\|v\|_{\mathcal{Y}}^2 \; = \; \boldsymbol{v}^T \, \boldsymbol{\mathcal{Y}} \, \boldsymbol{v}$

The dual norm of the residual is then

$$\|r(\cdot; y_N(\mu), \mu)\|_{\mathcal{Y}'}^2 \; = \; (\boldsymbol{f}(\mu) - \boldsymbol{\mathcal{A}}(\mu)\boldsymbol{y}_N(\mu))^T \, \boldsymbol{\mathcal{Y}}^{-1}(\boldsymbol{f}(\mu) - \boldsymbol{\mathcal{A}}(\mu)\boldsymbol{y}_N(\mu))$$

Simplest Case: Poisson Problem

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Let $\|v\|_{\mathcal{Y}}^2 \;=\; \boldsymbol{v}^T \, \boldsymbol{\mathcal{Y}} \, \boldsymbol{v}$

The dual norm of the residual is then

$$\begin{aligned}
\|r(\cdot; y_N(\mu), \mu)\|_{\mathcal{Y}'}^2 \;&=\; (\boldsymbol{f}(\mu) - \boldsymbol{\mathcal{A}}(\mu)\boldsymbol{y}_{N}(\mu))^T \, \boldsymbol{\mathcal{Y}}^{-1}(\boldsymbol{f}(\mu) - \boldsymbol{\mathcal{A}}(\mu)\boldsymbol{y}_{N}(\mu)) \\
&=\; \boldsymbol{f}^T\boldsymbol{\mathcal{Y}}^{-1}\boldsymbol{f} - 2\boldsymbol{f}^T\boldsymbol{\mathcal{Y}}^{-1}\boldsymbol{\mathcal{A}}\,\boldsymbol{y}_{N} + (\boldsymbol{\mathcal{A}}\,\boldsymbol{y}_{N})^T \, \boldsymbol{\mathcal{Y}}^{-1}\boldsymbol{\mathcal{A}}\,\boldsymbol{y}_{N}
\end{aligned}$$

Simplest Case: Poisson Problem

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&= \boldsymbol{f}^T\boldsymbol{\mathcal{Y}}^{-1}\boldsymbol{f} - 2\boldsymbol{f}^T\boldsymbol{\mathcal{Y}}^{-1}\boldsymbol{\mathcal{A}}\,\boldsymbol{y}_N + (\boldsymbol{\mathcal{A}}\,\boldsymbol{y}_N)^T\,\boldsymbol{\mathcal{Y}}^{-1}\boldsymbol{\mathcal{A}}\,\boldsymbol{y}_N \\
&= \ldots + \left(\sum_{q=1}^{Q} \theta_a^q(\mu)\boldsymbol{\mathcal{A}}^q\boldsymbol{\mathcal{W}}_N\boldsymbol{y}_N(\mu)\right)^T \boldsymbol{\mathcal{Y}}^{-1}\left(\sum_{q'=1}^{Q} \theta_a^{q'}(\mu)\boldsymbol{\mathcal{A}}^{q'}\boldsymbol{\mathcal{W}}_N\boldsymbol{y}_N(\mu)\right)
\end{aligned}$$

which permits a similar offline-online decomposition

Simplest Case: Poisson Problem

General Form	Matrix Form
Find $y(\mu) \in \mathcal{Y}$ s.t. $a(y(\mu), v; \mu) = f(v; \mu) \quad \forall\, v \in \mathcal{Y}$	Find $\boldsymbol{y}_{\mathcal{N}}(\mu) \in \mathbb{R}^{\mathcal{N}}$ s.t. $\boldsymbol{\mathcal{A}}_{\mathcal{N}}(\mu)\boldsymbol{y}_{\mathcal{N}}(\mu) = \boldsymbol{f}_{\mathcal{N}}(\mu)$, where $\boldsymbol{\mathcal{A}}_{\mathcal{N}} \in \mathbb{R}^{\mathcal{N}\times\mathcal{N}}$, $\boldsymbol{f}_{\mathcal{N}} \in \mathbb{R}^{\mathcal{N}}$

Questions:

How can we compute an approximation $y_N(\mu)$ to $y(\mu)$?

How do we know the error is small?

How do we know what value of N to take?

How do we compute $y_N(\mu)$, $s_N(\mu)$ efficiently online?

How do we choose the sample points μ_i optimally?

Simplest Case: Poisson Problem

How can we choose the snapshots optimally?

Greedy algorithm

Given the samples $S = \{\mu_1, ..., \mu_N\}$ and space of snapshots

$\mathcal{Y}_N = \mathrm{span}\{\ y(\mu_i)\ ,\ i = 1, \ldots, N\ \}$, we want to choose

$$\mu_{N+1} \;=\; \max_{\mu \in \mathcal{D}} \frac{\|y(\mu) - y_N(\mu)\|_{\mathcal{Y}}}{\|y(\mu)\|_{\mathcal{Y}}}$$

Simplest Case: Poisson Problem

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Given the samples $S = \{\mu_1, ..., \mu_N\}$ and space of snapshots

$\mathcal{Y}_N = \mathrm{span}\{\ y(\mu_i)\ ,\ i = 1, \ldots, N\ \}$, we want to choose

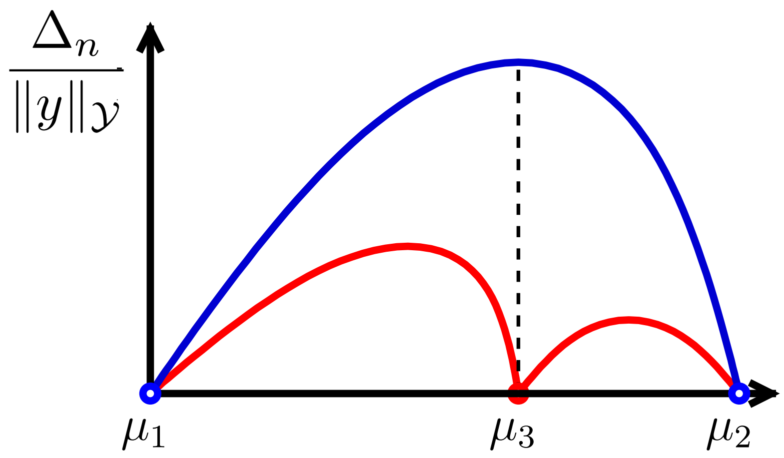
$$\mu_{N+1} \;=\; \max_{\mu \in \mathcal{D}} \frac{\|y(\mu) - y_N(\mu)\|_{\mathcal{Y}}}{\|y(\mu)\|_{\mathcal{Y}}}$$

In practice, we choose

$$\mu_{N+1} \;=\; \max_{\underbrace{\mu \in D}_{\text{training sample}}} \frac{\overbrace{\Delta_N(\mu)}^{\text{error bound}}}{\|\underbrace{y_N(\mu)}_{\text{approximation}}\|_{\mathcal{Y}}}$$

(Weak) Greedy Algorithm

Given $\mathcal{Y}_2 = \text{span}\{y(\mu_1), y(\mu_2)\}$, how do we choose μ_3?



$$\mu_3 = \arg\max_{\mu \in D} \frac{\Delta_2(\mu)}{\|u_2(\mu)\|_{\mathcal{Y}}}$$

$$\mathcal{Y}_3 = \text{span}\{u(\mu_1),\ u(\mu_2),\ u(\mu_3)\}$$

(see, e.g., [VEROY, et al., 2003], [BINEV, et al., 2011])

Key points:

- $\Delta_N(\mu)$ is sharp and inexpensive to compute (online)
- Error bounds enable choice of good approximation spaces

Simplest Case: Poisson Problem

Algorithm: Offline

Choose training sample $D \subset \mathcal{D}$ and first snapshot parameter $\mu_1 \in D$.

For $N = 1 \text{ to } N_{\max}$

Solve $a(y(\mu_N), v; \mu_N) = f(v; \mu_N), \quad \forall\, v \in \mathcal{Y}.$

Compute and store for $q, q' = 1, ..., Q$

$$\mathbf{A}_N^q = \boldsymbol{\mathcal{W}}_N^T \boldsymbol{\mathcal{A}}^q \boldsymbol{\mathcal{W}}_N, \qquad \boldsymbol{\Gamma}_N^{qq'} = (\boldsymbol{\mathcal{A}}^q \boldsymbol{\mathcal{W}}_N)^T \boldsymbol{\mathcal{Y}}^{-1} (\boldsymbol{\mathcal{A}}^{q'} \boldsymbol{\mathcal{W}}_N)^T$$

and other μ-independent quantities

Find $\mu_{N+1} = \arg\max_{\mu \in D} \dfrac{\Delta_N(\mu)}{\|\boldsymbol{y}_N(\mu)\|_{\mathcal{Y}}}$

Set $N = N + 1$

end

Simplest Case: Poisson Problem

Algorithm: Online

For given $\mu \in \mathcal{D}$,

Assemble $\mathbf{A}_N(\mu) \;=\; \sum_{q=1}^{Q_a} \theta_a^q(\mu)\mathbf{A}_N^q$ and, similarly, $\mathbf{f}_N(\mu)$

Solve $\mathbf{A}_N(\mu)\,\mathbf{y}_N(\mu) \;=\; \mathbf{f}_N(\mu)$.

Compute $\alpha_a^{\mathrm{LB}}(\mu)$,

$$\|r(\cdot; y_N(\mu), \mu)\|_{\mathcal{Y}'}^2 \;=\; \ldots + \sum_{q,q'}^{Q_a} \mathbf{y}_N^T(\mu)\,\mathbf{\Gamma}_N^{qq'}\mathbf{y}_N(\mu)$$

and $\Delta_N(\mu) \;=\; \dfrac{\|r(\cdot; y_N(\mu), \mu)\|_{\mathcal{Y}'}}{\alpha_a^{\mathrm{LB}}(\mu)}$.

Simplest Case

What about the output of interest?

Assume $s(\mu) = f(y(\mu))$.

Then $s_N(\mu) = f(y_N(\mu)) = \boldsymbol{y}_N^T(\mu)\boldsymbol{f}_{\mathcal{N}}$

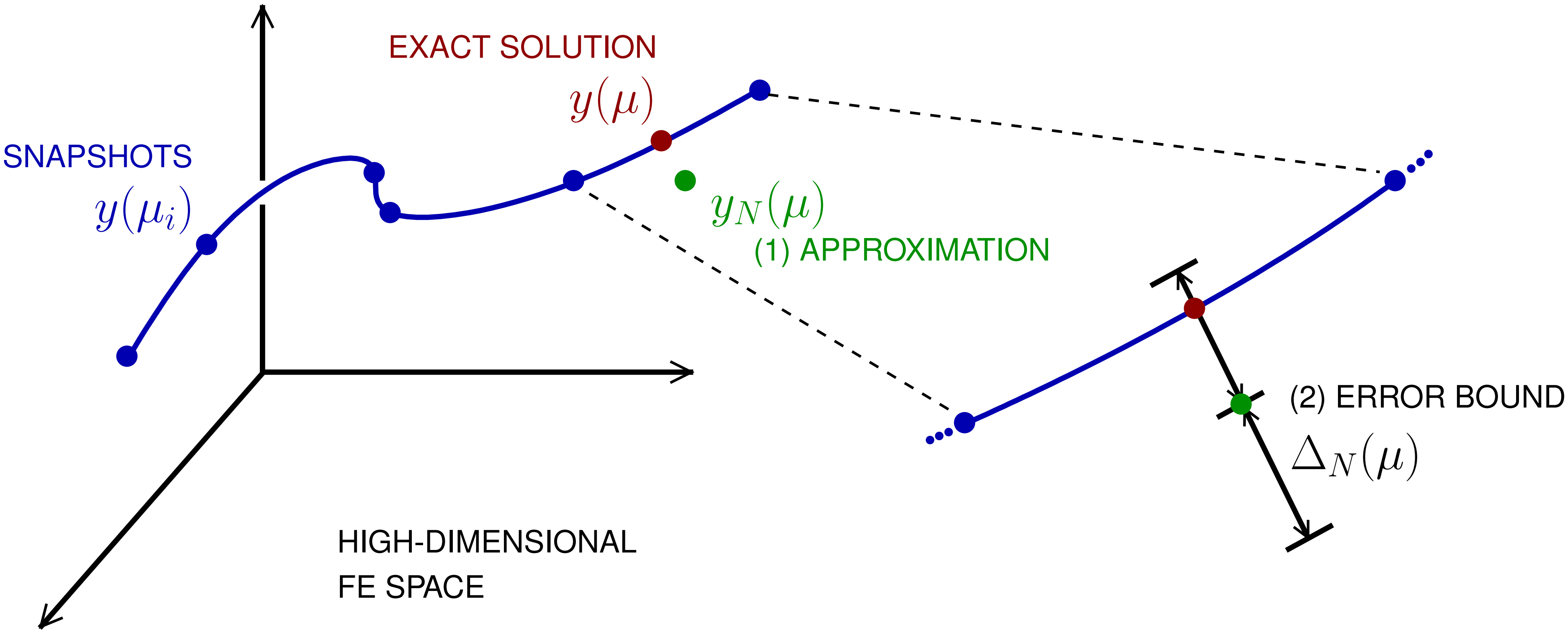
$$= \underbrace{\mathbf{y}_N^T(\mu)}_{\text{online}} \underbrace{(\boldsymbol{\mathcal{W}}_N^T \boldsymbol{f}_{\mathcal{N}})}_{\text{offline}}$$

One can show that for

$$s - s_N(\mu) \leq \frac{\|r(\cdot; y_N(\mu); \mu)\|_{\mathcal{Y}'}^2}{\alpha_a^{\mathrm{LB}}(\mu)}$$

which also permits an offline-online decomposition.

The Reduced Basis Method



(3) OFFLINE-ONLINE COMPUTATIONAL DECOMPOSITION
(4) GREEDY ALGORITHM

Simplest Case

Problem: Compute $s(\mu) = f(y(\mu); \mu)$ where

$$a(u(\mu), v; \mu) = f(v; \mu), \qquad \forall\, v \in \mathcal{Y},$$

where f is a bounded linear form.

a is a coercive, continuous bilinear form.

a, f are affine in μ .

What about more complex cases?

More Complex Cases

Part I: Introduction to the Reduced Basis Method

- Simplest Case (Coercive, Compliant, Elliptic, Affine)
- **Noncompliant**
- **Parabolic**
- **Noncoercive**
- **Saddle Point**
- **Non-affine / Non-linear**

Noncompliant Problems

Noncompliant Case

Problem: Compute $s(\mu) = \ell(y(\mu);\mu)$ where

$$a(y(\mu), v; \mu) = f(v;\mu), \qquad \forall\, v \in \mathcal{Y}$$

with $\ell \neq f$.

One can show that

$$\begin{aligned} |s(\mu) - s_N(\mu)| &= \ell(y(\mu) - y_N(\mu);\mu) \\ &\leq \|\ell(\cdot;\mu)\|_{\mathcal{Y}'} \|y(\mu) - y_N(\mu)\|_{\mathcal{Y}} \\ &\leq \|\ell(\cdot;\mu)\|_{\mathcal{Y}'} \Delta_N(\mu) \end{aligned}$$

Noncompliant Case

One can also show that

$$|s(\mu) - s_N(\mu)| \leq \frac{1}{\alpha_a^{\mathrm{LB}}(\mu)} \, \|r^{\mathrm{pr}}(\cdot; y_N(\mu), \mu)\|_{\mathcal{Y}'} \, \|r^{\mathrm{du}}(\cdot; \psi_N(\mu), \mu)\|_{\mathcal{Y}'}$$

where r^{pr} is the primal residual (as before), and the dual residual is

$$r^{\mathrm{du}}(v; \mu) \ := \ -l(v; \mu) - a(v, \psi_N(\mu); \mu) \qquad \forall\, v \in \mathcal{Y}$$

and $\psi_N(\mu) \in \mathcal{Y}_N^{\mathrm{du}}$ approximates $\psi(\mu) \in \mathcal{Y}$ where

$$a(v, \psi(\mu); \mu) \ = \ -l(v; \mu), \qquad \forall\, v \in \mathcal{Y}$$

Parabolic Problems

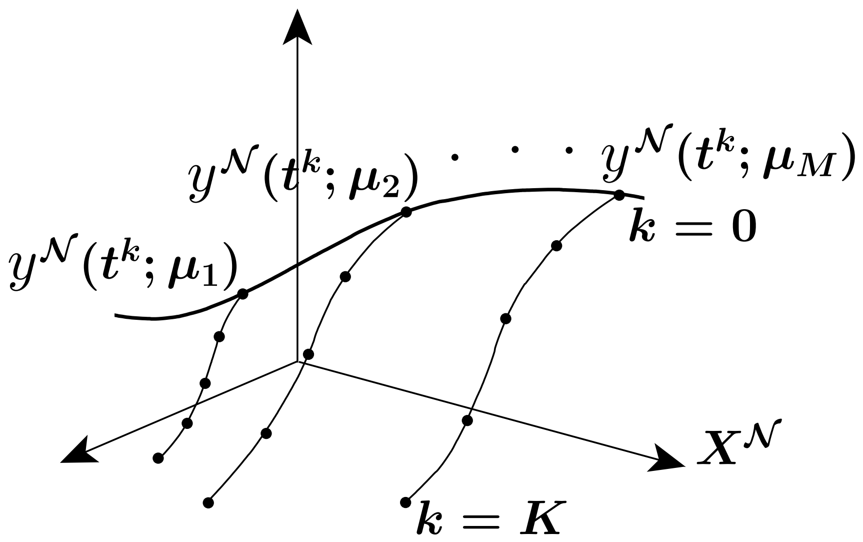
Parabolic Case

Problem: Given $\mu \in \mathcal{D}$, evaluate

$$s(t;\mu) \;=\; \ell(y(x,t;\mu);\mu)$$

where $y(x,t;\mu)$ satisfies $\qquad y^k \;=\; y(x,t^k;\mu)$

$$m\left(\frac{y^k - y^{k-1}}{\Delta t}, v; \mu\right) + a(y,v;\mu) \;=\; f(v;\mu)g(t)$$



We assume that m and a are

- symmetric
- continuous
- coercive

bilinear forms for all $\mu \in \mathcal{D}$.

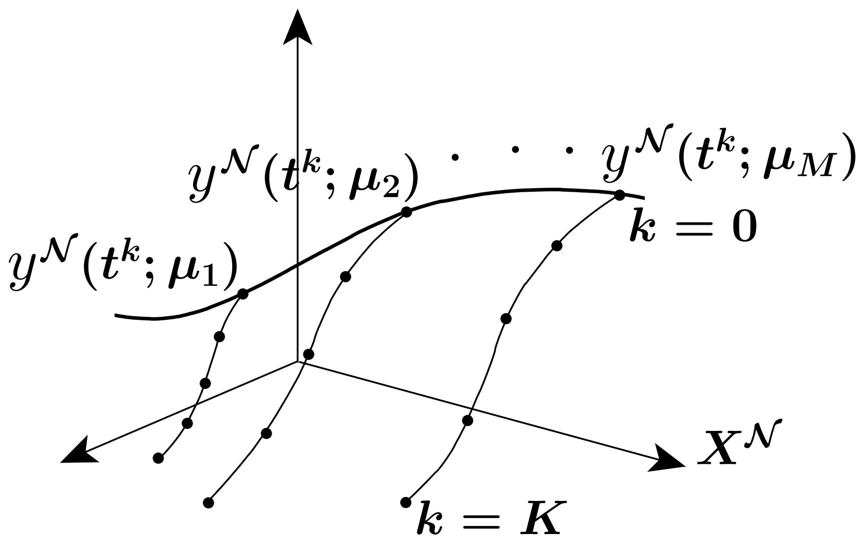
Parabolic Case

For a given $\mu_i \in \mathcal{D}$, let

$$P_R \;=\; \mathrm{POD}_{\mathcal{Y}}(\{y^k(\mu), 1 \le k \le K\}, R)$$

represent the R largest POD modes with respect to the $\mathcal{Y}$-inner product, s.t.

$$P_R \;=\; \arg\inf_{\mathcal{Y}_R \subset \mathrm{span}\{y^k, k=1\ldots K\}} \left(\frac{1}{k} \sum_{k=1}^{K} \inf_{v \in X_R} \|y^k(\mu) - v\|^2_{\mathcal{Y}} \right)^{1/2}$$



- Compute an $\mathrm{SVD}_{\mathcal{Y}}$
- Choose largest mode(s).
- In practice, do POD on error instead of directly on data.

Noncoercive Problems

Noncoercive Problems

Problem: Find $y(\mu) \in \mathcal{Y}$ such that

$$a(y(\mu), v; \mu) \;=\; f(v; \mu), \quad \forall\, v \in \mathcal{Y}$$

Assume that

$$\beta(\mu) \;=\; \inf_{w \in \mathcal{Y}} \sup_{v \in \mathcal{Y}} \frac{a(w, v; \mu)}{\|w\|_{\mathcal{Y}} \|v\|_{\mathcal{Y}}} \geq \beta_0 > 0$$

RB Approximation: Find $y_N(\mu) \in \mathcal{Y}_N$ such that

$$a(y_N(\mu), v; \mu) \;=\; f(v; \mu), \quad \forall\, v \in \mathcal{Y}_N$$

Is the RB Problem well-posed?

Noncoercive Problems

Problem: Find $y \in \mathcal{Y}_1$ such that

$$a(y, v) \;=\; f(v) \quad \forall\, v \in \mathcal{Y}_2$$

where $a: \; \mathcal{Y}_1 \times \mathcal{Y}_2 \to \mathbb{R}$ is a continuous bilinear form

$f: \; \mathcal{Y}_2 \to \mathbb{R}$ is a continuous linear functional

Noncoercive Problems

Problem: Find $y \in \mathcal{Y}_1$ such that

$$a(y, v) \;=\; f(v) \quad \forall\, v \in \mathcal{Y}_2$$

where $a: \; \mathcal{Y}_1 \times \mathcal{Y}_2 \to \mathbb{R}$ is a continuous bilinear form

$f: \; \mathcal{Y}_2 \to \mathbb{R}$ is a continuous linear functional

Banach-Nečas-Babuška Thm: The problem is well-posed if and only if:

$$\exists\, \beta_o > 0 \text{ such that } \inf_{w \in \mathcal{Y}_1} \sup_{v \in \mathcal{Y}_2} \frac{a(w, v)}{\|w\|_{\mathcal{Y}_1} \|v\|_{\mathcal{Y}_2}} \geq \beta_o$$

(BNB1) $\mathrm{Ker}\{\mathrm{A}\} = 0$

$$\forall\, v \in \mathcal{Y}_2 \quad (a(w, v) = 0, \;\; \forall\, w \in \mathcal{Y}_1) \Rightarrow (v = 0)$$

(BNB2) $\mathrm{Ker}\{\mathrm{A}^{\mathrm{T}}\} = 0$

Moreover,

$$\|y\|_{\mathcal{Y}_1} \leq \frac{1}{\beta} \|f\|_{\mathcal{Y}_2'} \quad \forall\, f \in \mathcal{Y}_2'$$

Noncoercive Problems

Recall that

$$\alpha \;=\; \inf_{v \in \mathcal{Y}} \frac{a(v,v)}{\|v\|_{\mathcal{Y}}^2} \;=\; \min_{\boldsymbol{v} \in \mathbb{R}^{\mathcal{N}}} \frac{\boldsymbol{v}^T \boldsymbol{A} \boldsymbol{v}}{\boldsymbol{v}^T \boldsymbol{Y} \boldsymbol{v}}$$

In other words α is the minimum eigenvalue of

$$\boldsymbol{A}\boldsymbol{\varphi} \;=\; \boldsymbol{\lambda} \boldsymbol{Y} \boldsymbol{\varphi}$$

How can we interpret the inf-sup constant β?

Noncoercive Problems

Riesz Representation Theorem

Let $\mathcal{Y}$ be a Hilbert space, and $f \in \mathcal{Y}'$. Then there exists a unique element $p \in \mathcal{Y}$ such that

$$f(v) \; = \; (v, p)_{\mathcal{Y}} \quad \forall \, v \in \mathcal{Y}.$$

Furthermore

$$\|f\|_{\mathcal{Y}'} \; = \; \sup_{v \in \mathcal{Y}} \frac{f(v)}{\|v\|_{\mathcal{Y}}} \; = \; \|p\|_{\mathcal{Y}}$$

For given $w \in \mathcal{Y}$, let $f(v) = a(w, v)$ …

Noncoercive Problems

If a is continuous, then for a given $w \in \mathcal{Y}$,

- $a(w, \cdot) \in \mathcal{Y}'$
- there exists a unique element $\mathcal{T}_w \in \mathcal{Y}$ s.t.

$$(\mathcal{T}_w, v)_{\mathcal{Y}} = a(w, v), \quad \forall v \in \mathcal{Y}$$

- furthermore

$$\mathcal{T}_w = \arg \sup_{v \in \mathcal{Y}} \frac{a(w, v)}{\|v\|_{\mathcal{Y}}}$$

Noncoercive Problems

If a is continuous, then for a given $w \in \mathcal{Y}$,

- $a(w, \cdot) \in \mathcal{Y}'$
- there exists a unique element $\mathcal{T}_w \in \mathcal{Y}$ s.t.

$$(\mathcal{T}_w, v)_{\mathcal{Y}} = a(w, v), \quad \forall v \in \mathcal{Y}$$

- furthermore

$$\mathcal{T}_w = \arg \sup_{v \in \mathcal{Y}} \frac{a(w,v)}{\|v\|_{\mathcal{Y}}}$$

In matrix form, $\boldsymbol{\mathcal{Y}} \boldsymbol{\mathcal{T}}_w = \boldsymbol{\mathcal{A}} \boldsymbol{w}$ or $\boldsymbol{\mathcal{T}}_w = \boldsymbol{\mathcal{Y}}^{-1} \boldsymbol{\mathcal{A}} \boldsymbol{w}$

Noncoercive Problems

Recall that

$$\beta(\mu) = \inf_{w \in \mathcal{Y}} \sup_{v \in \mathcal{Y}} \frac{a(w, v; w)}{\|w\|_{\mathcal{Y}} \|v\|_{\mathcal{Y}}} = \inf_{w \in \mathcal{Y}} \frac{1}{\|w\|_{\mathcal{Y}}} \left(\sup_{v \in \mathcal{Y}} \frac{a(w, v; \mu)}{\|v\|_{\mathcal{Y}}} \right)$$

$$= \inf_{w \in \mathcal{Y}} \frac{a(w, T_w; \mu)}{\|w\|_{\mathcal{Y}} \|T_w\|_{\mathcal{Y}}} = \frac{\|T_w\|_{\mathcal{Y}}}{\|w\|_{\mathcal{Y}}}$$

Noncoercive Problems

Recall that

$$\beta(\mu) = \inf_{w\in\mathcal{Y}} \sup_{v\in\mathcal{Y}} \frac{a(w,v;w)}{\|w\|_{\mathcal{Y}}\|v\|_{\mathcal{Y}}} = \inf_{w\in\mathcal{Y}} \frac{1}{\|w\|_{\mathcal{Y}}} \left(\sup_{v\in\mathcal{Y}} \frac{a(w,v;\mu)}{\|v\|_{\mathcal{Y}}} \right)$$

$$= \inf_{w\in\mathcal{Y}} \frac{a(w,T_w;\mu)}{\|w\|_{\mathcal{Y}}\|T_w\|_{\mathcal{Y}}} = \frac{\|T_w\|_{\mathcal{Y}}}{\|w\|_{\mathcal{Y}}}$$

In matrix form,

$$\boldsymbol{\beta}^2(\mu) = \min_{w\in\mathbb{R}^{\mathcal{N}}} \frac{\mathbf{w}^T\mathbf{A}(\mu)^T\mathbf{Y}^{-1}\mathbf{A}(\mu)\mathbf{w}}{\mathbf{w}^T\mathbf{Y}\mathbf{w}}$$

Noncoercive Problems

Recall that

$$\beta(\mu) = \inf_{w \in \mathcal{Y}} \sup_{v \in \mathcal{Y}} \frac{a(w, v; w)}{\|w\|_{\mathcal{Y}} \|v\|_{\mathcal{Y}}} = \inf_{w \in \mathcal{Y}} \frac{1}{\|w\|_{\mathcal{Y}}} \left(\sup_{v \in \mathcal{Y}} \frac{a(w, v; \mu)}{\|v\|_{\mathcal{Y}}} \right)$$

$$= \inf_{w \in \mathcal{Y}} \frac{a(w, T_w; \mu)}{\|w\|_{\mathcal{Y}} \|T_w\|_{\mathcal{Y}}} = \frac{\|T_w\|_{\mathcal{Y}}}{\|w\|_{\mathcal{Y}}}$$

In matrix form,

$$\boldsymbol{\beta}^2(\mu) = \min_{w \in \mathbb{R}^{\mathcal{N}}} \frac{\mathbf{w}^T \mathbf{A}(\mu)^T \mathbf{Y}^{-1} \mathbf{A}(\mu) \mathbf{w}}{\mathbf{w}^T \mathbf{Y} \mathbf{w}}$$

In other words, $\boldsymbol{\beta}^2(\mu)$ is the minimum eigenvalue of

$$\mathbf{A}(\mu)^T \mathbf{Y}^{-1} \mathbf{A}(\mu) \varphi = \lambda \mathbf{Y} \varphi$$

Noncoercive Problems

Problem: Find $y(\mu) \in \mathcal{Y}$ such that

$$a(y(\mu), v; \mu) \;=\; f(v; \mu), \quad \forall\, v \in \mathcal{Y}$$

Assume that

$$\beta(\mu) \;=\; \inf_{w \in \mathcal{Y}} \sup_{v \in \mathcal{Y}} \frac{a(w, v; \mu)}{\|w\|_{\mathcal{Y}} \|v\|_{\mathcal{Y}}} \geq \beta_0 > 0$$

RB Approximation: Find $y_N(\mu) \in \mathcal{Y}_N$ such that

$$a(y_N(\mu), v; \mu) \;=\; f(v; \mu), \quad \forall\, v \in \mathcal{Y}_N$$

Is the RB Problem well-posed?

Noncoercive Problems

One can show that for

$$\mathcal{Y}_N := \mathrm{span}\{\, y(\mu_1), \ldots, y(\mu_N) \,\},$$

$$\mathcal{V}_N^\mu := \mathrm{span}\{\, T_\mu y(\mu_n),\ n = 1, \ldots, N \,\},$$

where

$$(\, T_\mu y(\mu_n), v \,)_{\mathcal{Y}} = a(y(\mu_n), v; , \mu), \quad \forall v \in \mathcal{Y}$$

then the following reduced basis problem:

Find $y_N(\mu) \in \mathcal{Y}_N$ such that

$$a(y_N(\mu), v; \mu) \;=\; f(v; \mu), \quad \forall\, v \in \mathcal{V}_N^\mu$$

is well-posed with $\beta_N(\mu) \geq \beta(\mu)$.

Saddle Point Problems

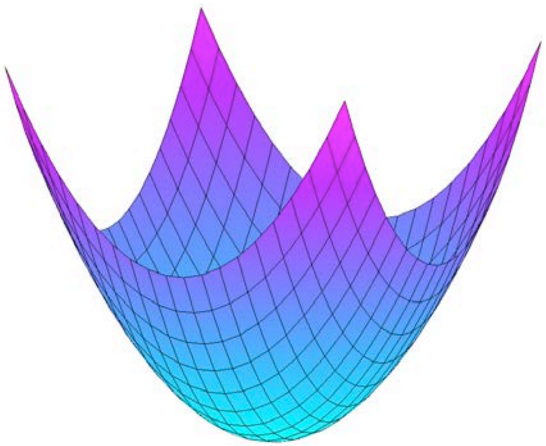
with

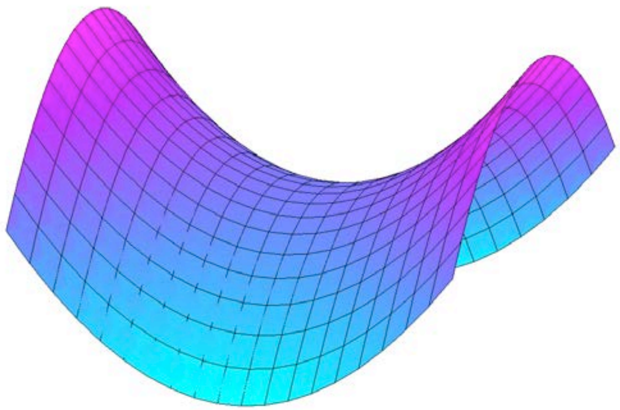
A.-L. Gerner

Saddle Point Problems

Problem Structure

$$\mathbf{A}\,\mathbf{y} = \mathbf{f} \qquad \text{vs.} \qquad \underbrace{\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix}}_{\boldsymbol{\mathcal{A}}\, U = \boldsymbol{\mathcal{F}}}$$



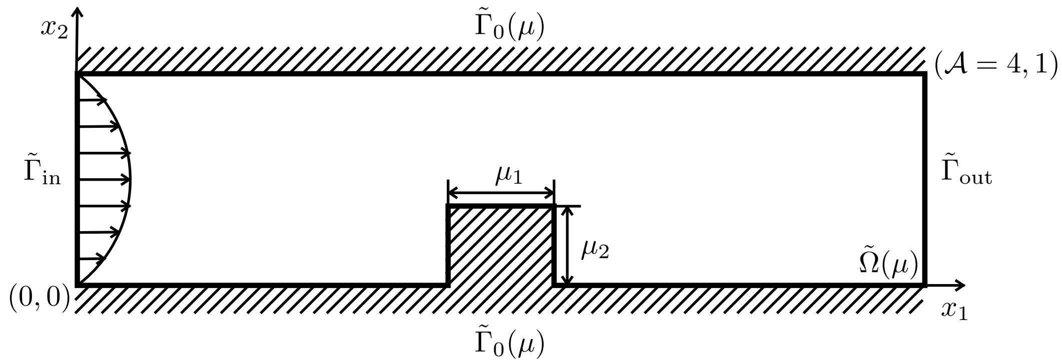


Saddle Point Problems

Applications

- Mixed finite element methods
- Optimization and optimal control

Example: **Stokes flow**



[GERNER & VEROY, 2012]

Saddle Point Problems

RB Approximation

Find $(y_N, \lambda_N) \in \mathcal{Y}_N \times \mathcal{Z}_N$ such that $\qquad (\mu)$

$$\begin{array}{lclcll} \langle A y_N, v\rangle & + & \langle B v, \lambda_N\rangle & = & \langle f, v\rangle & \forall\, v \in \mathcal{Y}_N \\ \langle B y_N, q\rangle & & & = & \langle g, q\rangle & \forall\, q \in \mathcal{Z}_N \end{array}$$

Issues:

- **Well-posedness** of the approximate problem
- Efficiently computable **bounds** for the errors

$$\|y - y_N\|_{\mathcal{Y}} \quad \text{and} \quad \|\lambda - \lambda_N\|_{\mathcal{Z}}$$

Saddle Point Problems

Status:

- **Approximation**

  — methods for construction of provably stable spaces

  but often requires many velocity basis functions

  [BREZZI, 1974]

  [ROVAS, 2003], [ROZZA & VEROY, 2007]

- **Error Estimation**

  — error bounds, but for the combined variable $Y = (y, \lambda)$

  and with high offline cost

  [VEROY, PRUD'HOMME, ROVAS & PATERA, 2003]

  [ROZZA, HUYNH & MANZONI, 2013]

Motivation:

- Construct stable *and* efficient approximation spaces
- Develop *separate* and offline-inexpensive error bounds

Saddle Point: Approximation

Status:

The spaces $\mathcal{Y}_N, \mathcal{Z}_N$ constitute a stable pair if for all $\mu \in \mathcal{D}$

$$\beta_N(\mu) := \inf_{q \in \mathcal{Z}_N} \sup_{v \in \mathcal{Y}_N} \frac{\langle B(\mu)v, q \rangle}{\|v\|_{\mathcal{Y}} \|q\|_{\mathcal{Z}}} > 0$$ [BREZZI]

For any $q \in \mathcal{Z}_N, \mathcal{Y}_N$ must contain “supremizing" functions.

Saddle Point: Approximation

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For any $q \in \mathcal{Z}_N, \mathcal{Y}_N$ must contain “supremizing" functions.

Pressure Space:

For $\mu_i \in \mathcal{D}$, $i = 1, \ldots, N$, and

$$\mathcal{Z}_N := \mathrm{span}\{\lambda(\mu_i),\ i = 1 \text{ to } N\}$$

Saddle Point: Approximation

Status:

The spaces $\mathcal{Y}_N, \mathcal{Z}_N$ constitute a stable pair if for all $\mu \in \mathcal{D}$

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[BREZZI]

For any $q \in \mathcal{Z}_N, \mathcal{Y}_N$ must contain “supremizing" functions.

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Velocity Space:

Option 0: The Naive Choice

$$\mathcal{Y}_N^0 := \operatorname{span}\{y(\mu_i),\ i = 1 \text{ to } N\}$$

Saddle Point: Approximation

Status:

The spaces $\mathcal{Y}_N, \mathcal{Z}_N$ constitute a stable pair if for all $\mu \in \mathcal{D}$

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For any $q \in \mathcal{Z}_N, \mathcal{Y}_N$ must contain “supremizing" functions.

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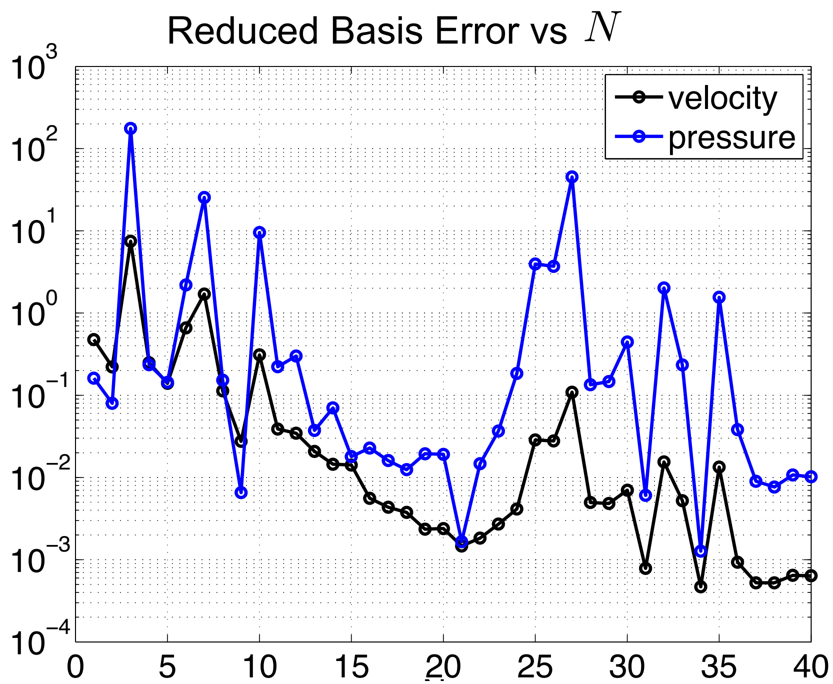


Saddle Point: Approximation

Velocity Space

For $i = 1, \ldots, N$ and $q = 1, \ldots, Q_b$

- **Option 1*** $\Rightarrow$ provably stable

*[ROVAS, 2003], [ROZZA & VEROY, 2007] †[GERNER & VEROY, 2012]

Saddle Point: Approximation

Velocity Space

For $i = 1, \dots, N$ and $q = 1, \dots, Q_b$

- **Option 1*** $\Rightarrow$ provably stable

$$\mathcal{Y}_N^1 := \text{span}\{\ y(\mu_i)\ ,\ T^q\lambda(\mu_i)\}$$

where

$$T^q p = \arg \sup_{v \in \mathcal{Y}_N} \frac{\langle B^q v, p\rangle}{\|v\|_{\mathcal{Y}}}$$

and

$$B(\mu) = \sum_{q=1}^{Q_b} \theta_b^q(\mu) B^q$$

*[ROVAS, 2003], [ROZZA & VEROY, 2007] † [GERNER & VEROY, 2012]

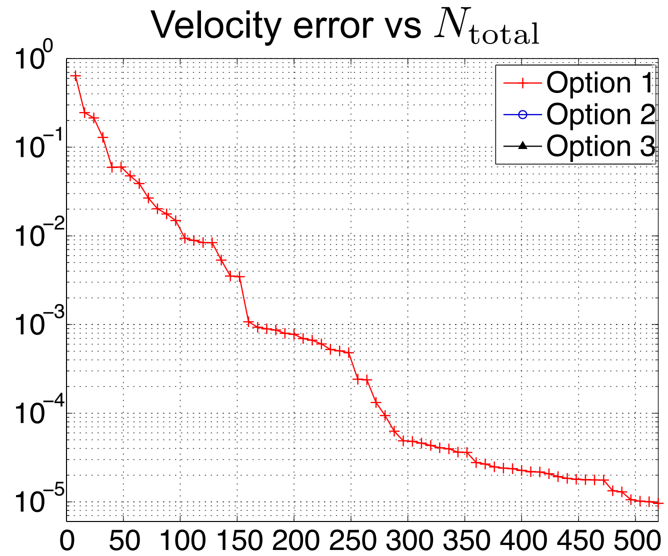
Saddle Point: Approximation

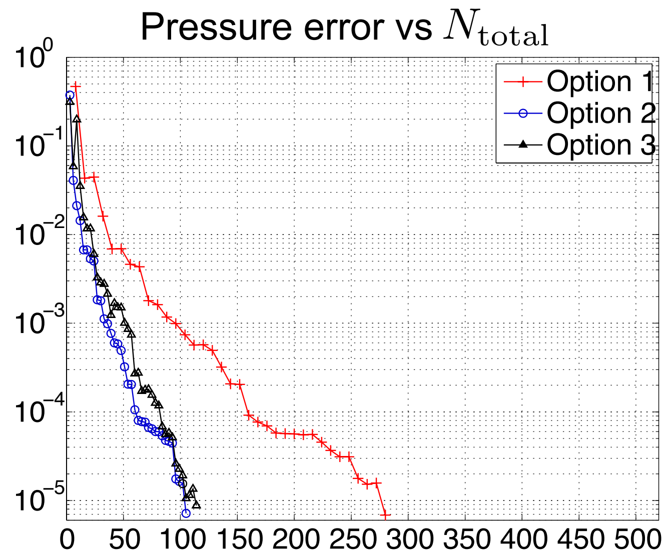
Velocity Space

For $i = 1, \dots, N$ and $q = 1, \dots, Q_b$

- **Option 1*** $\Rightarrow$ provably stable

$$\mathcal{Y}_N^1 := \text{span}\{\ y(\mu_i)\ ,\ \underbrace{T^q \lambda(\mu_i)}_{Q_b \text{ SUPREMIZERS}}\ \}$$





*[ROVAS, 2003], [ROZZA & VEROY, 2007] † [GERNER & VEROY, 2012]

Saddle Point: Approximation

Velocity Space

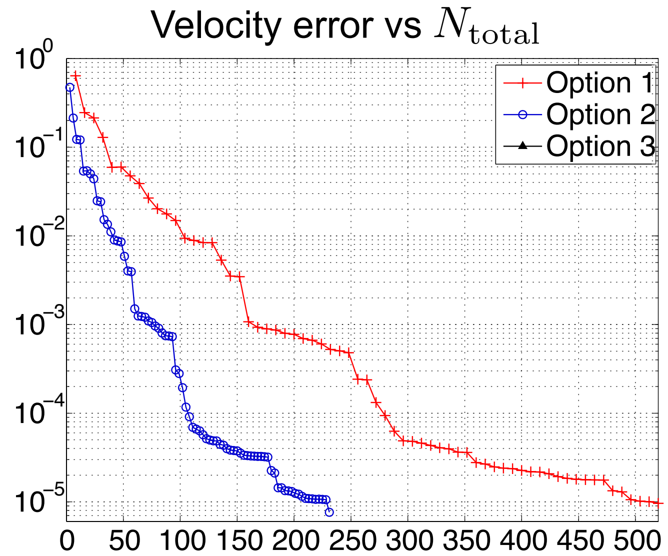
For $i = 1, \ldots, N$ and $q = 1, \ldots, Q_b$

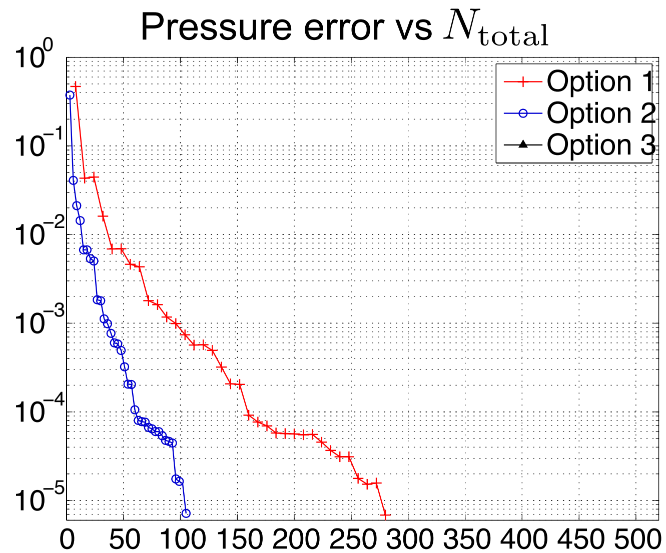
- **Option 1*** $\Rightarrow$ provably stable

$$\mathcal{Y}_N^1 := \text{span}\{\; y(\mu_i)\;,\; \underbrace{T^q \lambda(\mu_i)}_{Q_b \text{ SUPREMIZERS}} \;\}$$

- **Option 2**[†] $\Rightarrow$ justifiably stable

$$\mathcal{Y}_N^2 := \text{span}\{\; y(\mu_i)\;,\; \underbrace{T_{\mu_i} \lambda(\mu_i)}_{\text{SUPREMIZER SNAPSHOTS}} \;\}$$





*[ROVAS, 2003], [ROZZA & VEROY, 2007] †[GERNER & VEROY, 2012]

Saddle Point: Approximation

Velocity Space

For $i = 1, \ldots, N$ and $q = 1, \ldots, Q_b$

- **Option 1*** $\Rightarrow$ provably stable

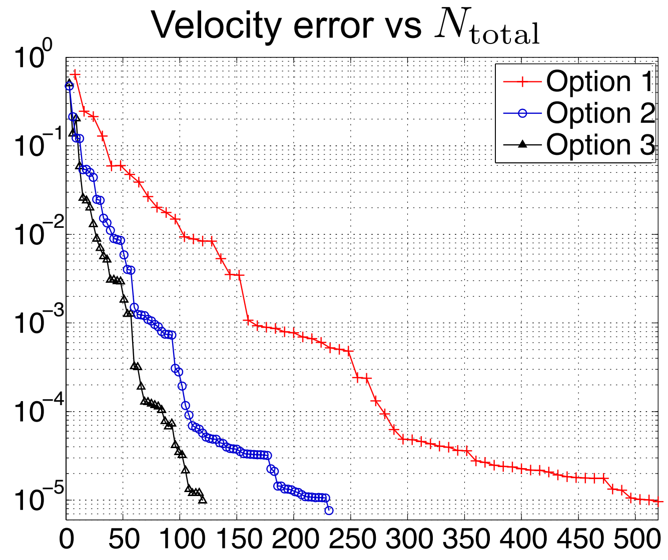
$$\mathcal{Y}_N^1 := \text{span}\{\ y(\mu_i)\ ,\ \underbrace{T^q \lambda(\mu_i)}_{Q_b \text{ SUPREMIZERS}}\ \}$$

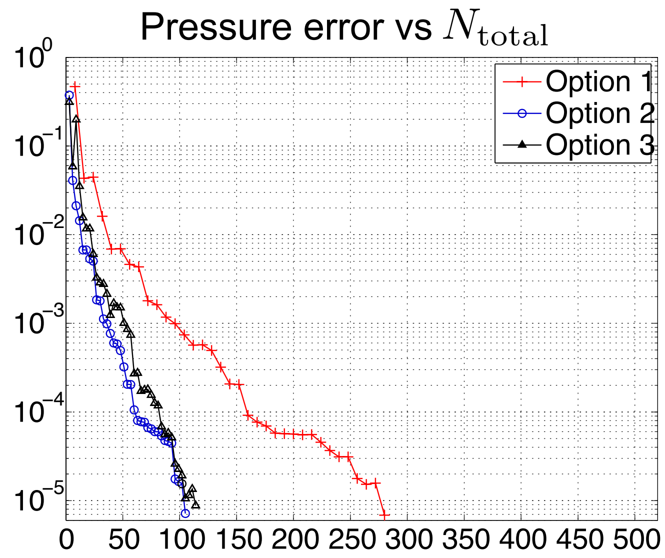
- **Option 2**† $\Rightarrow$ justifiably stable

$$\mathcal{Y}_N^2 := \text{span}\{\ y(\mu_i)\ ,\ \underbrace{T_{\mu_i} \lambda(\mu_i)}_{\text{SUPREMIZER SNAPSHOTS}}\ \}$$

- **Option 3**† $\Rightarrow$ empirically stable

$$\mathcal{Y}_N^3 := \text{span}\{y(\mu_i),\ \underbrace{y(\mu_i')}_{\text{VELOCITY SNAPSHOTS}}\ \}$$





*[ROVAS, 2003], [ROZZA & VEROY, 2007] †[GERNER & VEROY, 2012]

Saddle Point: Error Estimation

1. Treat entire system as a general noncoercive problem

$$\mathcal{A}(U(\mu), V; \mu) = \mathcal{F}(V; \mu), \quad \forall\, V \in \mathcal{X}$$

Let $\mathcal{R}(V;\mu)$ be the residual, [BANACH-NECAS-BABUSKA]

$$\|U(\mu) - U_N(\mu)\|_{\mathcal{X}} \leq \frac{\|\mathcal{R}(\,\cdot\,;\mu)\|_{\mathcal{X}'}}{\beta_{\mathrm{LB}}^{\mathrm{A}}(\mu)} =: \Delta_N^U(\mu)$$

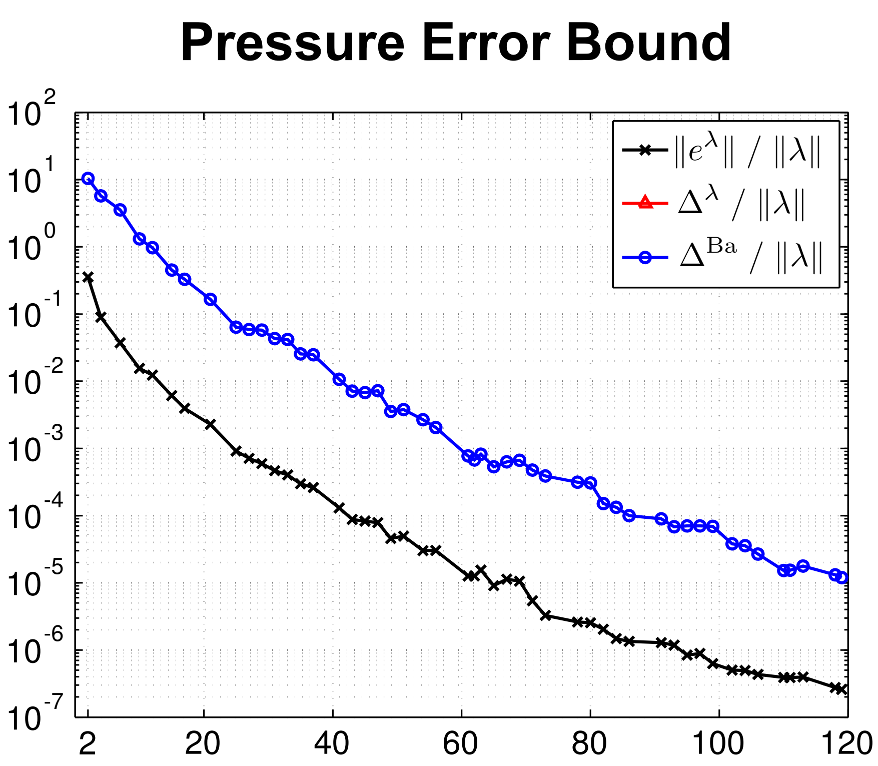
[VEROY, PRUD'HOMME, ROVAS & PATERA, 2003]
and, e.g., [ROZZA, HUYNH & MANZONI, 2013]

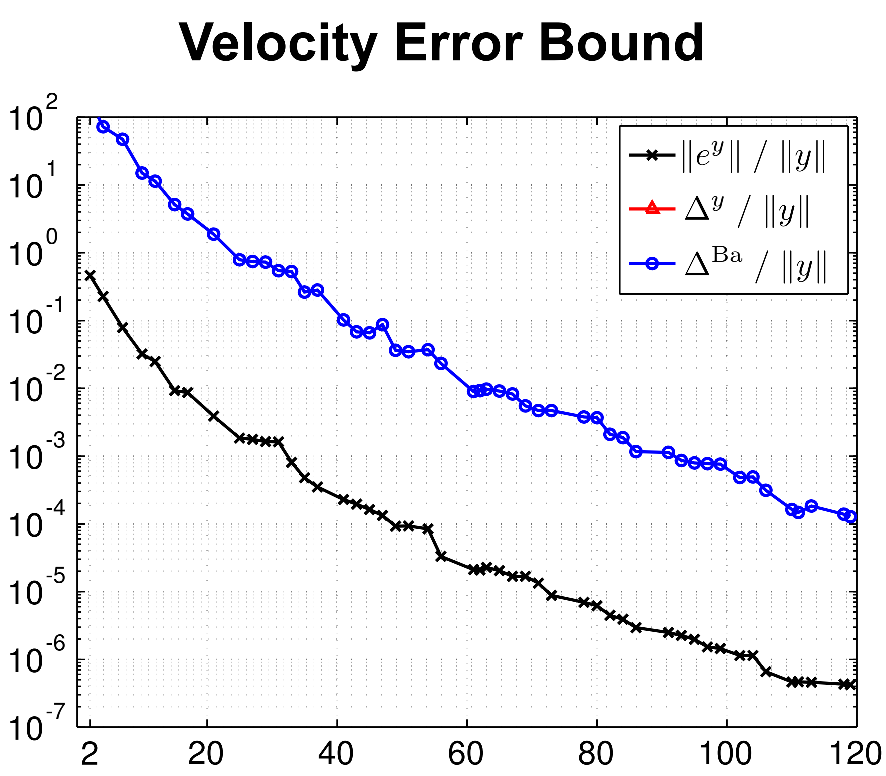
2. Treat the system as a saddle point problem [BREZZI]

$$\begin{aligned}
\|y - y_N\|_{\mathcal{X}} \quad &\leq \quad \frac{\|r_N^1\|_{\mathcal{X}'}}{\alpha_{\mathrm{LB}}} + \left(1 + \frac{\gamma_{\mathrm{UB}}}{\alpha_{\mathrm{LB}}}\right)\frac{\|r_N^2\|_{\mathcal{X}'}}{\beta_{\mathrm{LB}}^b} \quad &=:\ \Delta_N^y \\
\|\lambda - \lambda_N\|_{\mathcal{X}} \quad &\leq \quad \frac{\|r_N^1\|_{\mathcal{X}'}}{\beta_{\mathrm{LB}}^b} + \frac{\gamma_{\mathrm{UB}}}{\beta_{\mathrm{LB}}^b}\Delta_N^y \quad &=:\ \Delta_N^\lambda
\end{aligned}$$

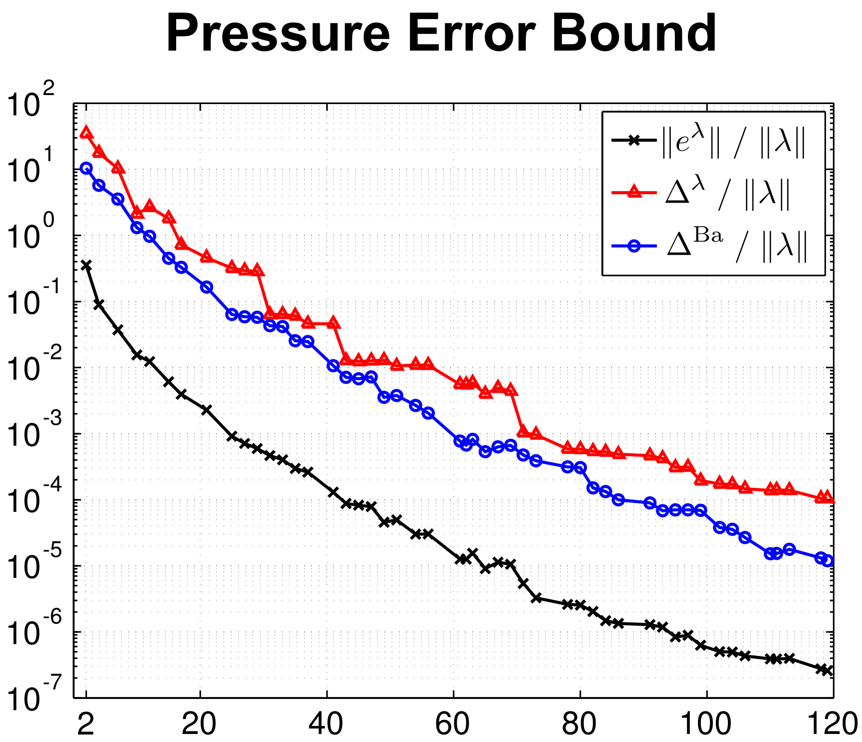
[GERNER & VEROY, 2012]

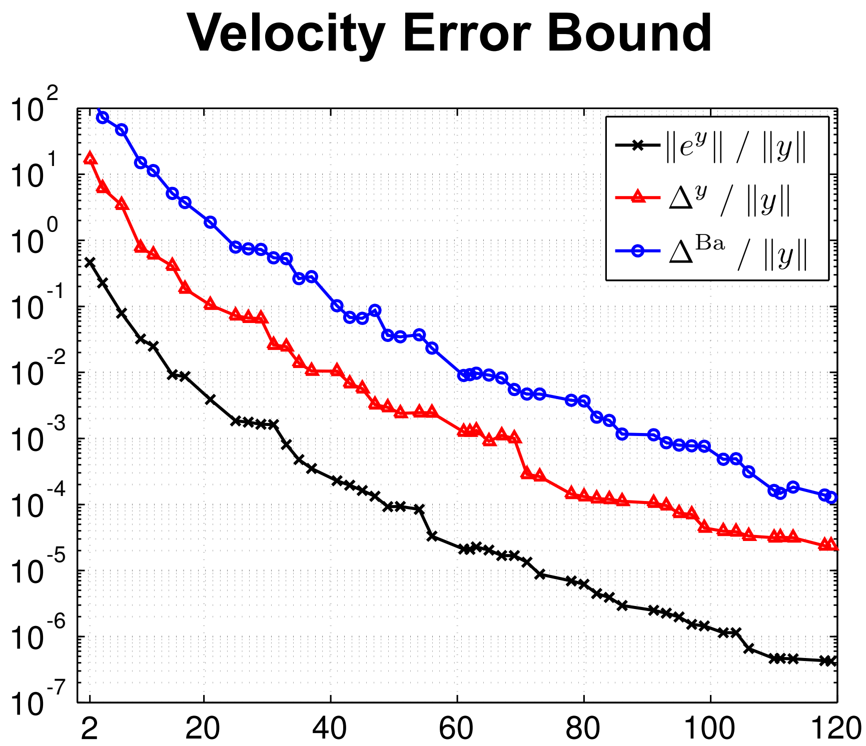
Saddle Point: Error Estimation





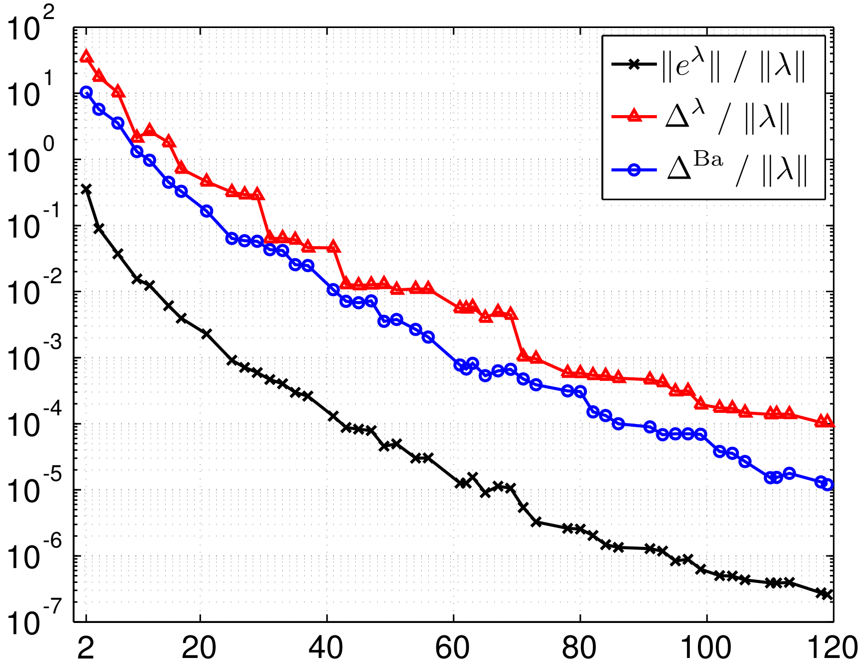
Saddle Point: Error Estimation



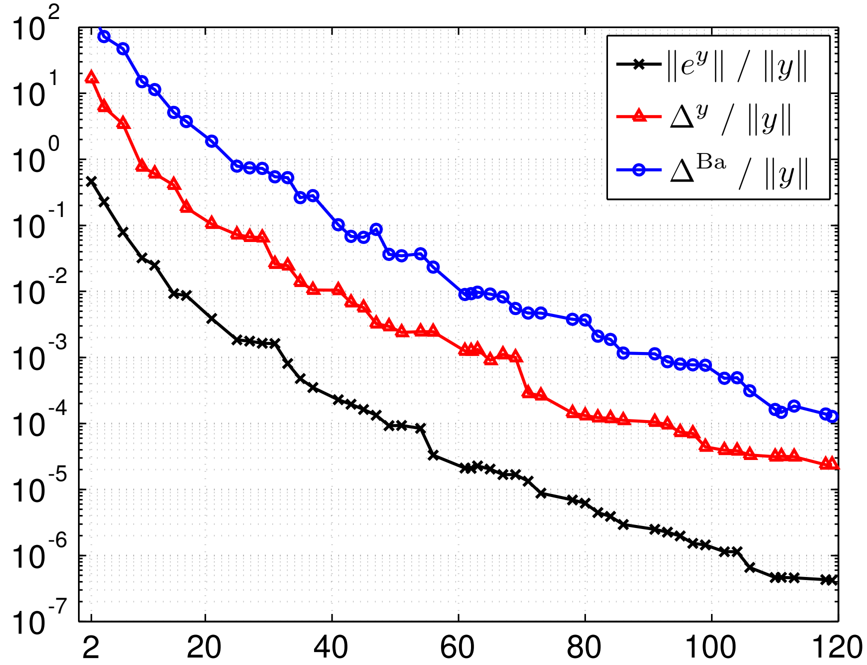


Saddle Point: Error Estimation

Pressure Error Bound



Velocity Error Bound



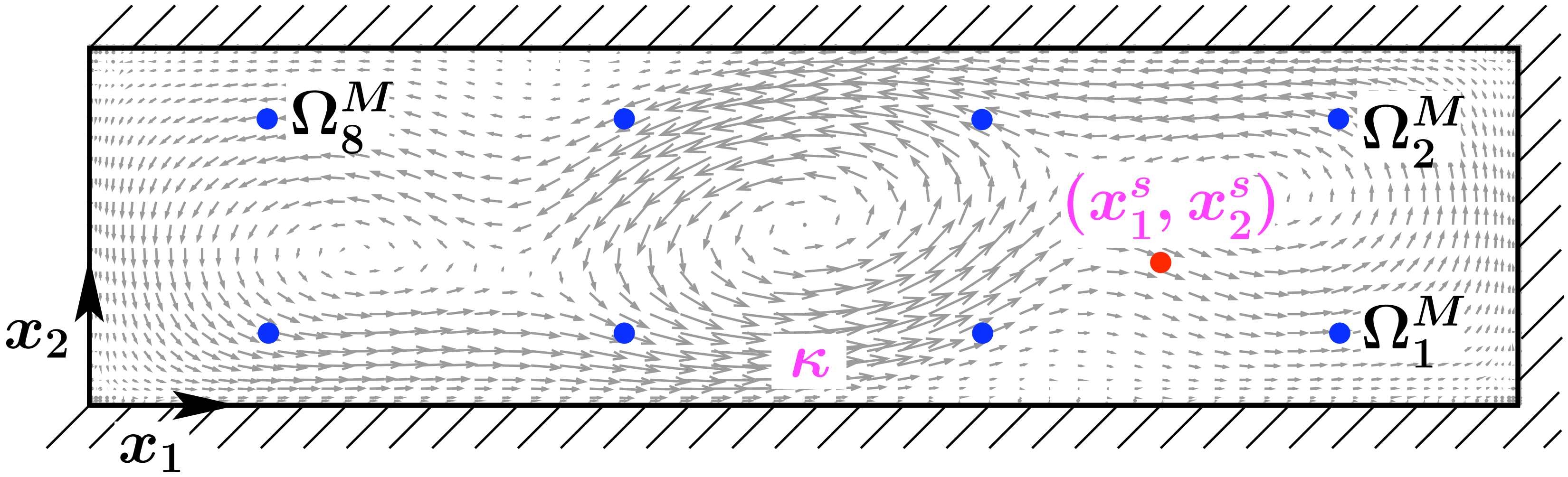
Key Result:

We provide separate error bounds for y_N, λ_N

that depend only on β^b, not on $\beta^{\mathcal{A}}$.

Non-Affine Problems

Contaminant Transport [Gre05]



Concentration $y(t;\mu)$ of pollutant in Ω governed by scalar convection-diffusion equation

$$\frac{\partial}{\partial t} y(t;\mu) + \mathbf{U} \cdot \nabla y(t;\mu) = \kappa\, \nabla^2 y(t;\mu) + g^{\mathrm{PS}}(x;\mu)\, g(t), \qquad y(x, t=0;\mu) = 0$$

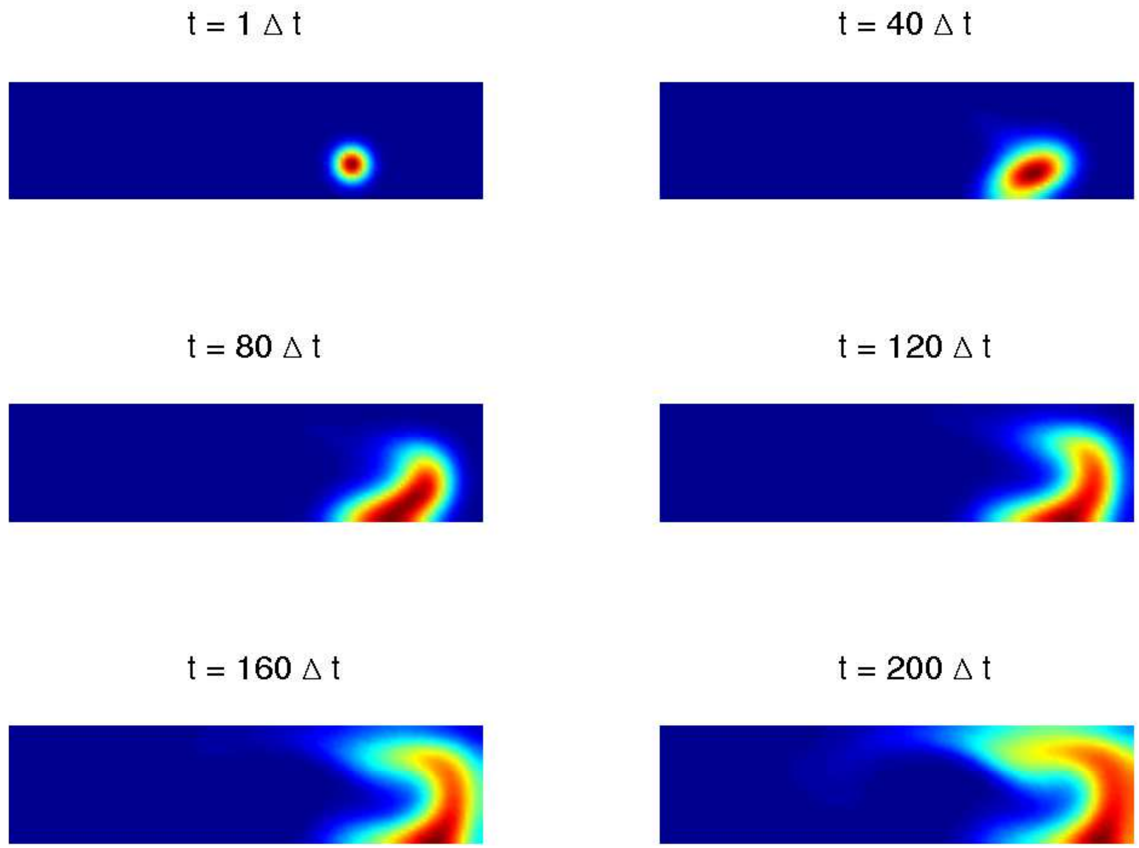
with source term modeled by

$$g^{\mathrm{PS}}(x;\mu) = \frac{50}{\pi}\, e^{-50((x_1 - x_1^s)^2 + (x_2 - x_2^s)^2)}.$$

Goal: Identify source location $\Rightarrow$ parameter $\mu \equiv (\kappa, x_1^s, x_2^s)$.

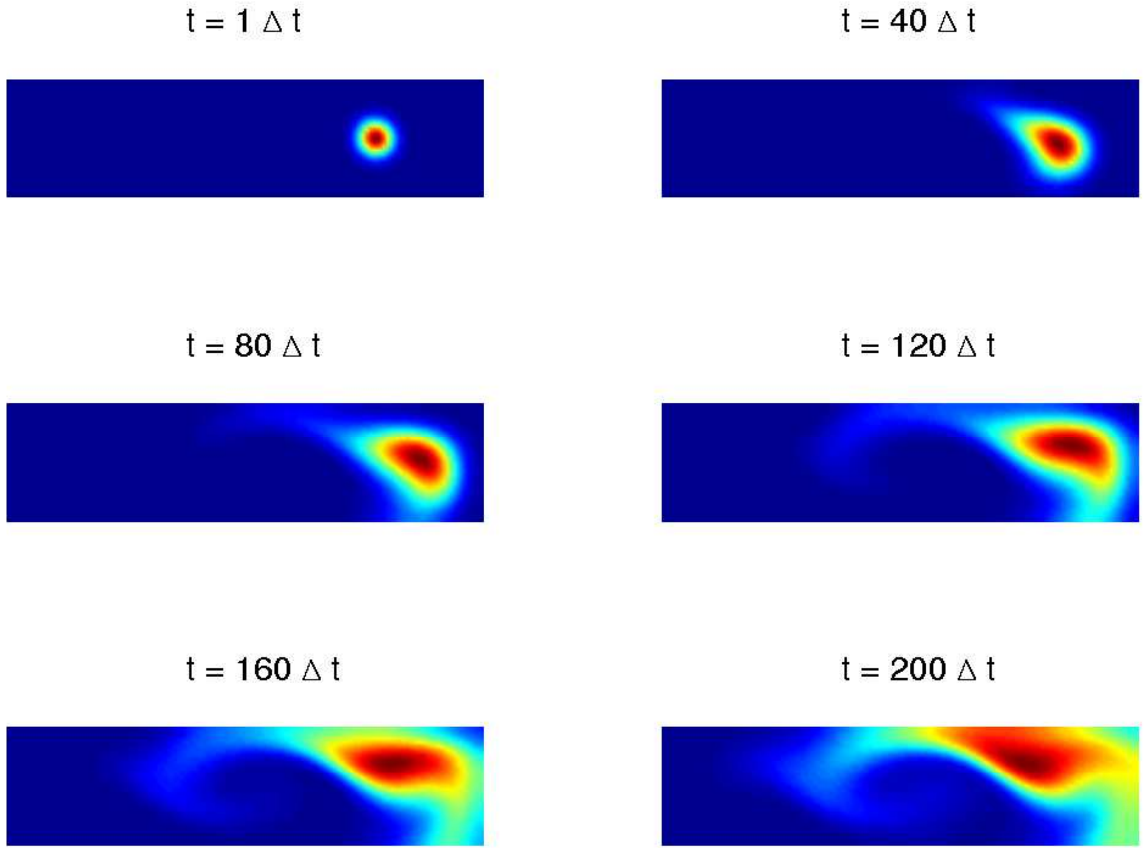
Contaminant Transport — Sample Solutions

Field variable: $\mu = (0.05, 2.9, 0.3)$ $(\mathbb{N} = 3720)$



Contaminant Transport — Sample Solutions

Field variable: $\mu = (0.05, 3.1, 0.5)$ $(\mathbb{N} = 3720)$



Contaminant Transport — Truth Problem Statement

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, evaluate $\forall k \in \mathbb{K}$

$$s(t^k;\mu) = \ell(y(t^k;\mu))$$

where $y(t^k;\mu) \in X$ satisfies $y(t^0;\mu) = 0$

$$m\left(\frac{y(t^k;\mu) - y(t^{k-1};\mu)}{\Delta t}, v; \mu\right) + \frac{1}{2}\, a(y(t^k;\mu) + y(t^{k-1};\mu), v; \mu)$$

$$= b(v;\mu)\, \frac{1}{2}\, (g(t^k) + g(t^{k-1})), \;\; \forall v \in X,$$

for $b(v;\mu) = \int_\Omega g^{\mathrm{PS}}(x;\mu)\, v\, d\Omega$ with g^{PS} nonaffine.

$$g^{\mathrm{PS}}(x;\mu) = \frac{50}{\pi}\, e^{-50((x_1 - x_1^s)^2 + (x_2 - x_2^s)^2)}.$$

Nonaffine Source Term

Evaluation of RB quantities $(v = \zeta_i,\ 1 \leq i \leq N_{\max})$:

$$
\begin{aligned}
b(\zeta_i;\mu) &= \int_\Omega g^{\mathrm{PS}}(x;\mu)\,\zeta_i \\
&= \frac{50}{\pi}\int_\Omega e^{-50((x_1-\mu_2)^2+(x_2-\mu_3)^2)}\,\zeta_i
\end{aligned}
$$

requires even in the online stage

$\mathcal{O}(\mathcal{N}N)$ operations.

Difficulty:

There is no ($\mathcal{N}$-independent) affine representation of $g^{\mathrm{PS}}(x;\mu)$.

Empirical Interpolation Method [BMNP04, GMNP07]

Main Idea

$$g^{\mathrm{PS}}(x;\mu) \approx g_M^{\mathrm{PS}}(x;\mu) = \sum_{m=1}^{M} \underbrace{\varphi_{Mm}(\mu)}_{\text{EIM}} \quad \underbrace{q_m(x)}_{\text{Collateral RB}}$$

Recall: $$b(\zeta_i;\mu) = \int_\Omega g^{\mathrm{PS}}(x;\mu)\,\zeta_i \approx \int_\Omega g_M^{\mathrm{PS}}(x;\mu)\,\zeta_i$$
$$= \sum_{m=1}^{M} \varphi_{Mm}(\mu) \int_\Omega q_m(x)\,\zeta_i \ ,$$

If we can calculate the $\varphi_{Mm}(\mu)$ efficiently, we can again follow an offline-online computational procedure, but

- how do we calculate the $q_m(x)$ and the $\varphi_{Mm}(\mu)$?
- what is the interpolation error introduced?

Greedy Approach [MNPP07]

Empirical Interpolation: Greedy approach for constructing both

- interpolation points $T_M = \{x_1^T \in \Omega, \ldots, x_M^T \in \Omega\}$ and
- sample set $S_M^g \equiv \{\mu_1^g \in \mathcal{D}, \ldots, \mu_M^g \in \mathcal{D}\}$ and associated discrete spaces $V_M^g = \mathrm{span}\{q_1, \ldots, q_M\}$.

Greedy Approach [MNPP07]

Empirical Interpolation: Greedy approach for constructing both

- interpolation points $T_M = \{\boldsymbol{x}_1^T \in \Omega, \ldots, \boldsymbol{x}_M^T \in \Omega\}$ and
- sample set $S_M^g \equiv \{\mu_1^g \in \mathcal{D}, \ldots, \mu_M^g \in \mathcal{D}\}$ and associated discrete spaces $V_M^g = \mathrm{span}\{q_1, \ldots, q_M\}$.

Greedy Procedure:

We first choose $\mu_1^g \in \mathcal{D}$ and compute

$$\xi_1 \equiv g(\boldsymbol{x}; \mu_1^g).$$

The first interpolation point is

$$\boldsymbol{x}_1 = \arg \max_{\boldsymbol{x} \in \Omega} |\xi_1(\boldsymbol{x})|$$

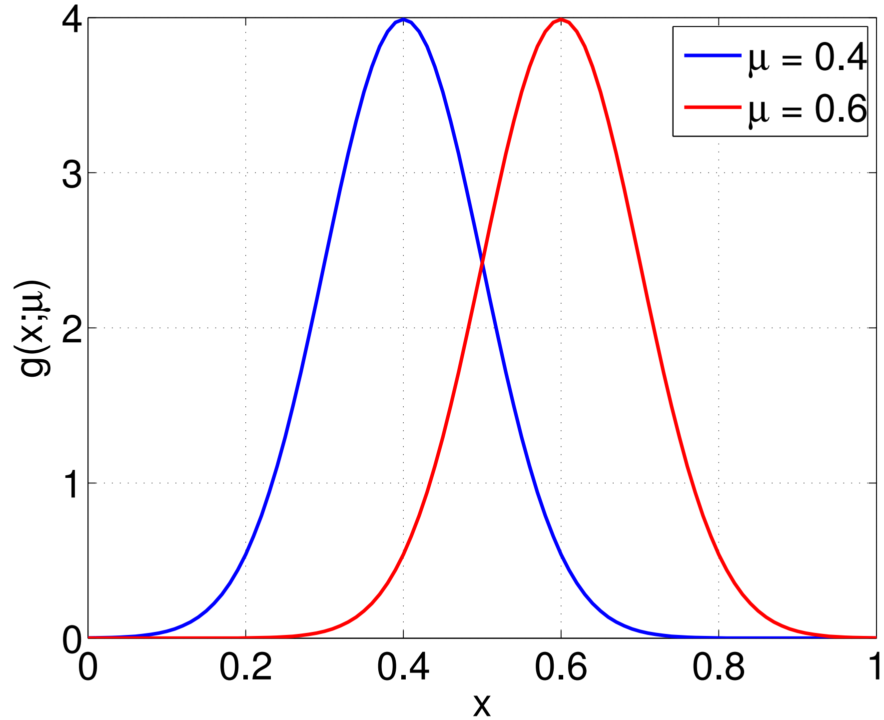
and we set $q_1 = \xi_1(\boldsymbol{x})/\xi_1(\boldsymbol{x}_1)$ and $B_{11}^1 = 1$.

Example / Demo

We consider the nonaffine function

$$g(x;\mu) \equiv \frac{10}{\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{0.1}\right)^2}$$

for $x \in \Omega \equiv [0,1]$ and $\mu \in \mathcal{D} \equiv [0.4, 0.6]$.



Greedy Approach

We then proceed by induction to generate S_M^g, W_M^g, and T_M:

For $1 \leq M \leq M_{\max}$, we first solve the interpolation problem

$$g_M(\boldsymbol{x}_i;\mu) = \sum_{j=1}^{M} B_{ij}^M \varphi_{M\,j}(\mu) = g(\boldsymbol{x}_i;\mu), \quad 1 \leq i \leq M,$$

where $B_{ij}^M = q_j(\boldsymbol{x}_i), 1 \leq i, j \leq M$, then compute

$$g_M(\boldsymbol{x};\mu) \equiv \sum_{m=1}^{M} \varphi_{M\,m}(\mu) q_m(\boldsymbol{x}),$$

and evaluate the interpolation error

$$\varepsilon_M(\mu) = \|g(\cdot;\mu) - g_M(\cdot;\mu)\|_{L^\infty(\Omega)}$$

for all $\mu \in \Xi_{\text{train}}^g$.

Greedy Approach

We then determine

$$\mu^g_{M+1} \equiv \arg \max_{\mu \in \Xi^g_{\text{train}}} \varepsilon_M(\mu)$$

and compute $\xi_{M+1} \equiv g(x; \mu^g_{M+1})$.

Greedy Approach

We then determine

$$\mu^g_{M+1} \equiv \arg \max_{\mu \in \Xi^g_{\text{train}}} \varepsilon_M(\mu)$$

and compute $\xi_{M+1} \equiv g(x; \mu^g_{M+1})$.

To generate the interpolation points we solve the linear system

$$\sum_{j=1}^{M} \sigma_j^M \, q_j(x_i) = \xi_{M+1}(x_i), \quad 1 \le i \le M$$

and we set $r_{M+1}(x) = \xi_{M+1}(x) - \sum_{j=1}^{M} \sigma_j^M \, q_j(x)$.

The next interpolation point is

$$x_{M+1} = \arg \max_{x \in \Omega} |r_{M+1}(x)|$$

and $q_{M+1}(x) = r_{M+1}(x)/r_{M+1}(x_{M+1})$.

A Posteriori Error Estimation

We have two options:

- Method 1: “Next Point” Estimator [BMNP04, GMNP07]
  - Very inexpensive to evaluate

    $\Rightarrow$ one additional evaluation of $g(x;\mu)$ at a single point in Ω.
  - In general not a rigorous upper bound for the error

    $\Rightarrow$ requires the saturation hypothesis.
- Method 2: Rigorous Estimator [EGP10]
  - Higher offline cost, since we require

    $\Rightarrow$ analytical upper bounds for parametric derivatives

    $\Rightarrow$ EIM approximation error at finite set of points in $\mathcal{D}$.
  - Provides rigorous upper bound for the error

Nonaffine "Truth" Problem Statement

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, evaluate $\qquad (\cdot) = (\cdot)^{\mathcal{N}}$

$$s(\mu) = \ell(y(\mu); \mu)$$

where $y(x;\mu) \in \mathcal{Y}$ satisfies

$$a(y(\mu), v; \mu) = f(v; g(x;\mu)), \quad \forall\, v \in \mathcal{Y}.$$

We consider the particular form

$$a(w, v; \mu) = a_0(w, v) + a_1(w, v; g(x;\mu)), \quad \forall w, v \in \mathcal{Y}.$$

where $g(x;\mu) \in L^\infty(\Omega)$ is nonaffine.

Hypotheses

We assume

- $a_0 \; : \mathcal{Y} \times \mathcal{Y} \to \mathrm{I\!R}$ is bilinear and parameter independent

$$a_0(w, v) = \int_\Omega \nabla w \, \nabla v, \quad \forall w, v \in \mathcal{Y}$$

- $a_1 \; : \mathcal{Y} \times \mathcal{Y} \times L^\infty(\Omega) \to \mathrm{I\!R}$ is trilinear

$$a_1(w, v, z) = \int_\Omega w \, v \, z, \quad \forall w, v \in \mathcal{Y}, \;\; z \in L^\infty(\Omega)$$

- and $f(v; g(x; \mu)) = \int_\Omega v \, g(x; \mu)$ is a linear form.

Coercivity & Continuity

We also assume that $a : \mathcal{Y} \times \mathcal{Y} \times \mathcal{D} \to \mathbb{R}$ is

- coercive

$$(0 <)\ \alpha(\mu) \equiv \inf_{w \in \mathcal{Y}} \frac{a(w,w;\mu)}{\|w\|_{\mathcal{Y}}^2};$$

- and continuous

$$\gamma(\mu) \equiv \sup_{w \in \mathcal{Y}} \sup_{v \in \mathcal{Y}} \frac{a(w,v;\mu)}{\|w\|_{\mathcal{Y}} \|v\|_{\mathcal{Y}}} \ (< \infty),$$

and that a_1 satisfies

$$a_1(w,v,z) \le \gamma_{a_1} \|w\|_{\mathcal{Y}} \, \|v\|_{\mathcal{Y}} \, \|z\|_{L^\infty(\Omega)}, \qquad \forall w, v \in \mathcal{Y},\ z \in L^\infty(\Omega).$$

Reduced Basis Sample and Space

Parameter samples:

$$S_N = \{\mu^1 \in \mathcal{D}, \ldots, \mu^N \in \mathcal{D}\}, \quad 1 \leq N \leq N_{\max},$$

with

$$S_1 \subset S_2 \subset \ldots \subset S_{N_{\max}-1} \subset S_{N_{\max}} \subset \mathcal{D}.$$

Lagrangian reduced basis spaces:

$$\mathcal{Y}_N = \text{span}\{ \underbrace{y(\mu^n)}_{\text{“snapshots”}}, 1 \leq n \leq N\}, \quad 1 \leq N \leq N_{\max},$$

with

$$\mathcal{Y}_1 \subset \mathcal{Y}_2 \subset \ldots \subset \mathcal{Y}_{N_{\max}-1} \subset \mathcal{Y}_{N_{\max}} (\subset \mathcal{Y}).$$

Reduced Basis Approximation

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, evaluate

$$s_{N,M}(\mu) = \ell(y_{N,M}(\mu); \mu)$$

where $y_{N,M}(x;\mu) \in \mathcal{Y}_N \subset \mathcal{Y}$ satisfies

$$a_0(y_{N,M}(\mu), v) + a_1(y_{N,M}(\mu), v; g_M(x;\mu)) = f(v; g_M(x;\mu)), \quad \forall\, v \in \mathcal{Y}_N.$$

where

$$g_M(x;\mu) \equiv \sum_{m=1}^{M} \varphi_{M\,m}(\mu) q_m(x),$$

and

$$\sum_{j=1}^{M} B_{ij}^M \varphi_{M\,j}(\mu) = g(x_i;\mu), \quad 1 \le i \le M.$$

Admits *offline-online* treatment: online cost $\mathcal{O}(M^2 + MN^2 + N^3)$

Error Residual Equation

The error, $e(\mu) \equiv y(\mu) - y_N(\mu) \in \mathcal{Y}$, satisfies

$$a_0(e(\mu), v) + a_1(e(\mu), v; g(x;\mu)) =$$

$$r(v;\mu) + f(v; g(x;\mu) - g_M(x;\mu))$$

$$-a_1(y_{N,M}(\mu), v; g(x;\mu) - g_M(x;\mu)),$$

$$\forall\, v \in \mathcal{Y},$$

where the residual is defined as

$$r(v;\mu) \equiv f(v; g_M(x;\mu))$$

$$-a_0(y_N(\mu), v) - a_1(y_N(\mu), v; g_M(x;\mu)),$$

$$\forall\, v \in \mathcal{Y}.$$

Energy Norm & Output Bound

Energy norm bound [Ngu07]

$$\Delta^y_{N,M}(\mu) = \frac{1}{\alpha_{\mathrm{LB}}(\mu)} \Bigg(\underbrace{\|r(\cdot;\mu)\|_{\mathcal{Y}'}}_{\text{affine}} + \underbrace{\hat{\varepsilon}_M(\mu)\Phi^{\mathrm{na}}_M(\mu)}_{\text{nonaffine}} \Bigg),$$

contribution to error bound

where

$\alpha_{\mathrm{LB}}(\mu)$	…	Lower bound of coercivity constant,
$\|r(\cdot;\mu)\|_{\mathcal{Y}'}$	…	dual norm of residual
$\hat{\varepsilon}_M(\mu)$	…	interpolation induced error

and

$$\Phi^{\mathrm{na}}_M(\mu) = \sup_{v\in\mathcal{Y}} \frac{f(v;q_{M+1}) - a_1(y_{N,M}, v; q_{M+1})}{\|v\|_{\mathcal{Y}}}$$

Output Error Bound

Note

- the output error bound:

$$\Delta^s_{N,M}(\mu) \equiv \|\ell(\cdot;\mu)\|_{\mathcal{Y}'}\, \Delta_{N,M}(\mu)$$

- and the output effectivity: $\eta^s_N(\mu) \equiv \dfrac{\Delta^s_N(\mu)}{|s(\mu) - s_N(\mu)|}$

Output Error Bound

Note

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- and the output effectivity: $\eta^s_N(\mu) \equiv \dfrac{\Delta^s_N(\mu)}{|s(\mu) - s_N(\mu)|}$

Proposition (Output Error Bound)

For any $N = 1, \ldots, N_{\max}$ *and any* $M = 1, \ldots, M_{\max}$ *, the error,* $|s(\mu) - s_N(\mu)|$*, satisfies*

$$|s(\mu) - s_N(\mu)| \leq \Delta^s_{N,M}(\mu), \qquad \forall \mu \in \mathcal{D}.$$

Model Problem

We consider the model problem with

$$g(x;\mu) \equiv \frac{1}{\sqrt{(x_1-\mu_{(1)})^2 + (x_2-\mu_{(2)})^2}}$$

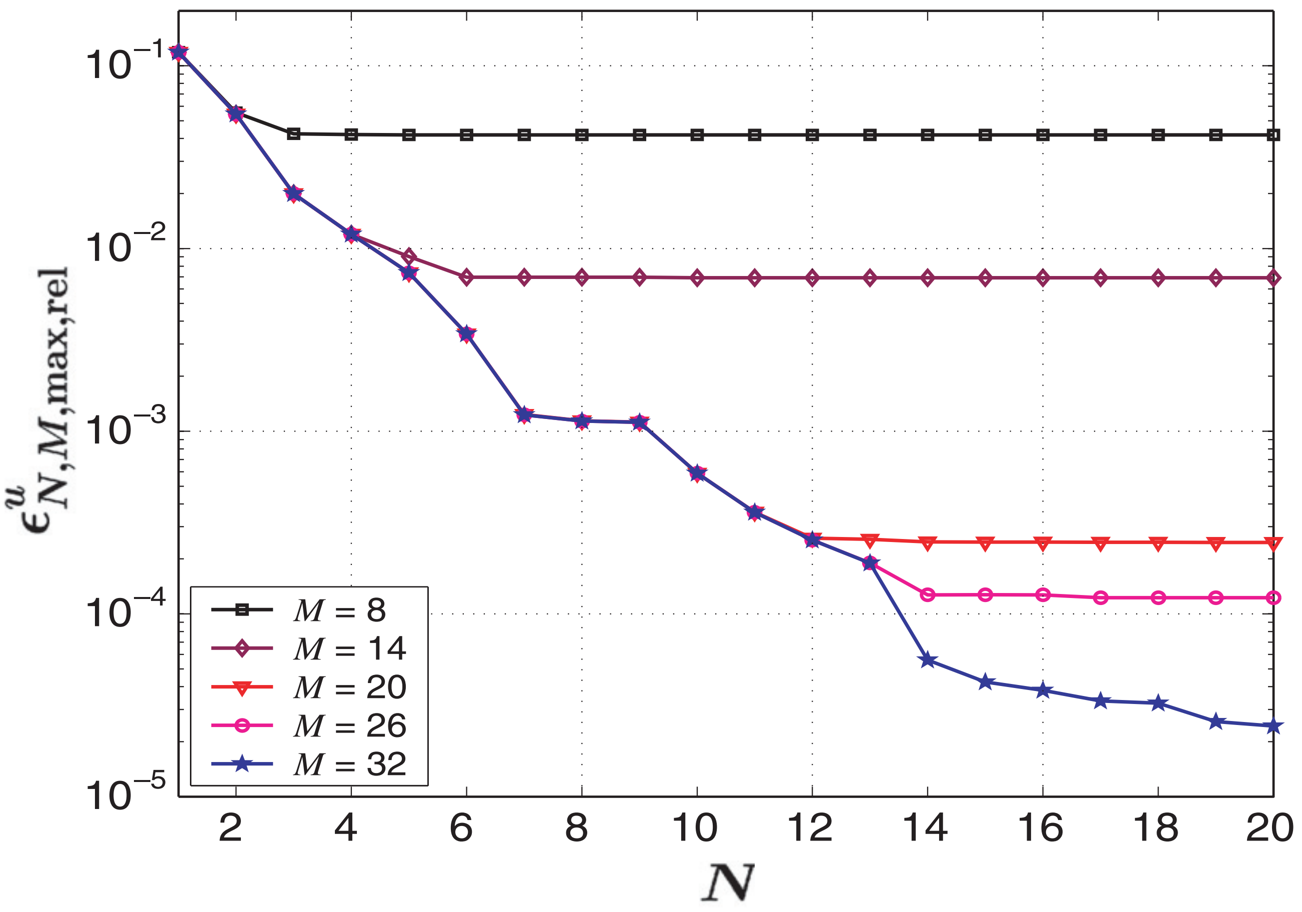
for $x \in \Omega \equiv \,]0,1[\,^2$ and $\mu \in \mathcal{D} \equiv [-1,-0.01]^2$.

Maximum relative error and bounds in field variable and output $[\mathrm{N}]$

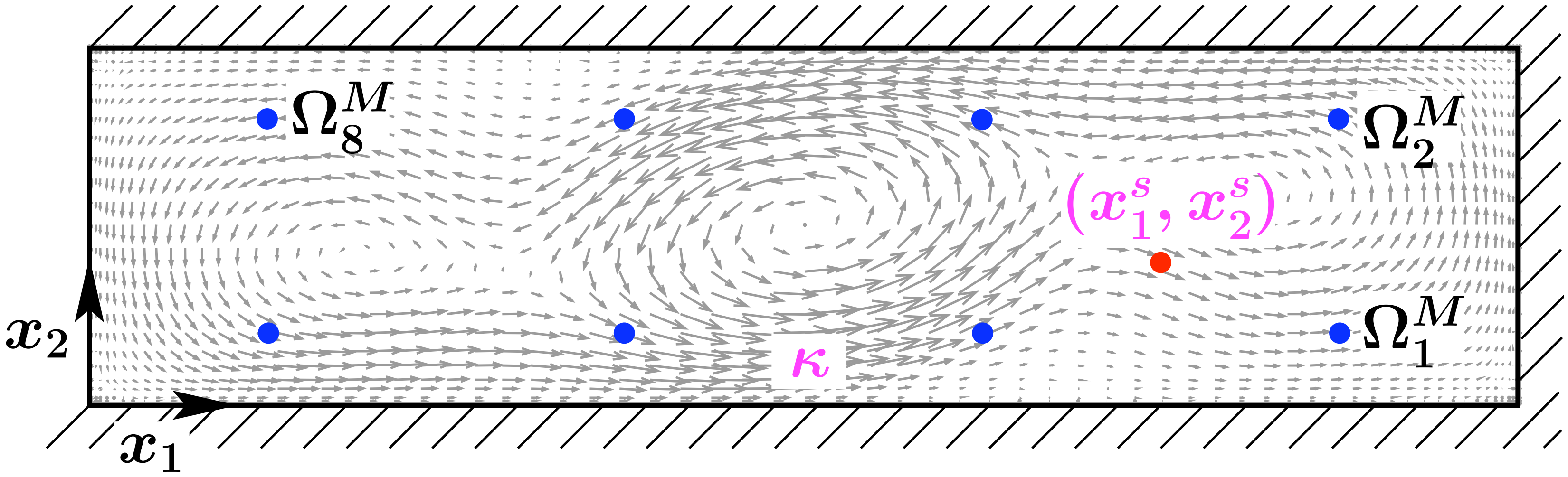
N	M	$\epsilon^u_{\mathrm{max,rel}}$	$\Delta^u_{\mathrm{max,rel}}$	$\bar{\eta}^u$	$\epsilon^s_{\mathrm{max,rel}}$	$\Delta^s_{\mathrm{max,rel}}$	$\bar{\eta}^s$
4	15	1.20E − 02	1.35E − 02	1.16	5.96E − 03	1.43E − 02	11.32
8	20	1.14E − 03	1.23E − 03	1.01	2.42E − 04	1.30E − 03	13.41
12	25	2.54E − 04	2.77E − 04	1.08	1.76E − 04	2.92E − 04	17.28
16	30	3.82E − 05	3.93E − 05	1.00	7.92E − 06	4.15E − 05	20.40

Model Problem

Maximum relative error in the field variable



Contaminant Transport



Concentration $y(t;\mu)$ of pollutant in Ω governed by scalar

convection-diffusion equation $\qquad y(x, t=0;\mu) = 0$

$$\frac{\partial}{\partial t} y(t;\mu) + \mathbf{U} \cdot \nabla y(t;\mu) = \kappa \nabla^2 y(t;\mu) + g^{\mathrm{PS}}(x;\mu)\, g(t),$$

with source term modeled by

$$g^{\mathrm{PS}}(x;\mu) = \frac{50}{\pi}\, e^{-50((x_1 - x_1^s)^2 + (x_2 - x_2^s)^2)}.$$

Goal: Identify source location $\Rightarrow$ parameter $\mu \equiv (\kappa, x_1^s, x_2^s)$.

Energy Norm & Output Bound

Energy norm bound [Gre05]

$$\Delta^{y\,k}_{N,M}(\mu) = \left\{ \frac{2\Delta t}{\alpha_{\mathrm{LB}}(\mu)} \left(\underbrace{\sum_{k'=1}^{k} \| r^{k'}_{N,M}(\cdot;\mu) \|^2_{\mathcal{Y}'}}_{\text{affine}} + \underbrace{\hat{\varepsilon}^2_M(\mu) \sum_{k'=1}^{k} \Phi^{\mathrm{na}}_M(t^{k'};\mu)^2}_{\text{nonaffine}} \right) \right\}^{\frac{1}{2}},$$

contribution to error bound

where $\alpha_{\mathrm{LB}}(\mu)$ … lower bound of coercivity constant,

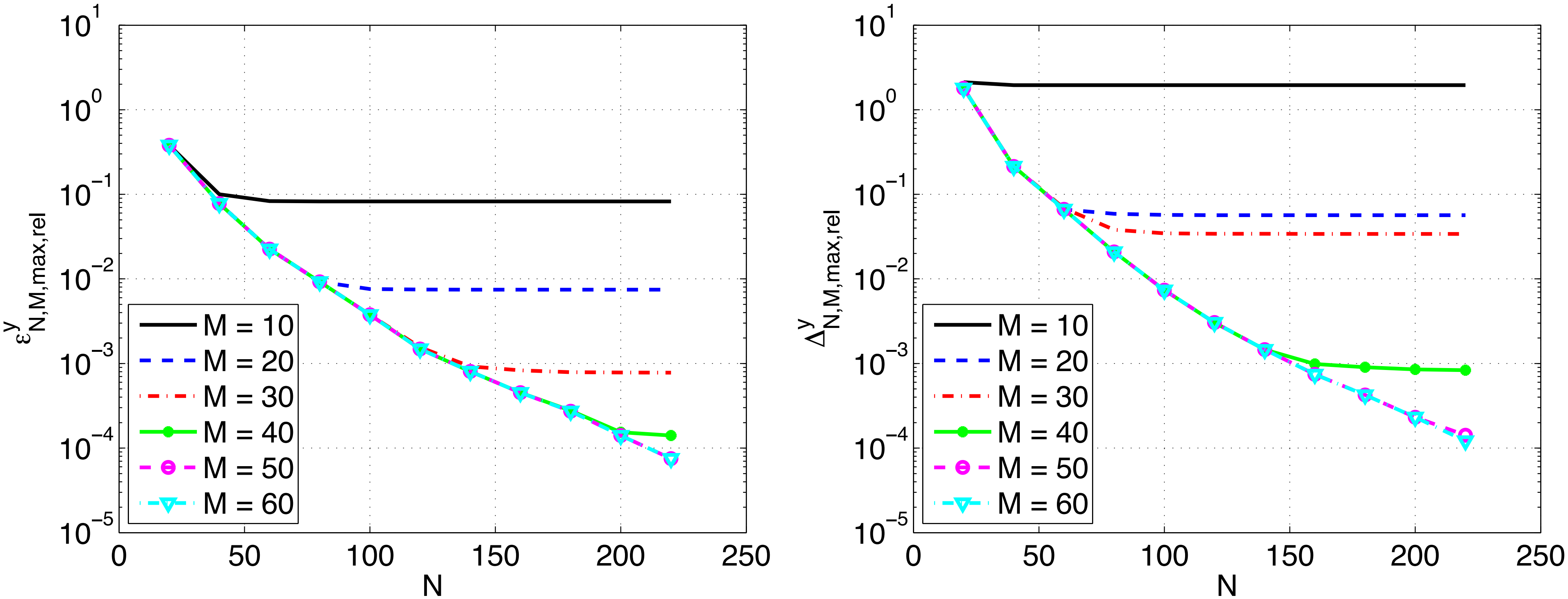
$\| r^{k}_{N,M}(\cdot;\mu) \|_{X'}$ … dual norm of residual

$\hat{\varepsilon}_M(\mu)$ … interpolation induced error.

Output bound

$$\Delta^{s\,k}_{N,M}(\mu) \equiv \left(\sup_{v \in Y} \frac{\ell(v)}{\|v\|_{L^2(\Omega)}} \right) \Delta^{y\,k}_{N,M}(\mu).$$

Contaminant Dispersion - Convergence: Energy Norm



Results for random sample $\Xi_{\mathbf{Test}} \in \mathcal{D}$ of size 2000.

Truth Problem Statement

Given $\mu \in \mathcal{D}$ evaluate $\quad \forall k \in \mathbb{K}$

$$s^k(\mu) = \ell(y^k(\mu))$$

where $y^k(\mu) \in \mathcal{Y}, 1 \leq k \leq K,$ satisfies $\quad y^0(\mu) = 0$

$$\frac{1}{\Delta t} m(y^k(\mu) - y^{k-1}(\mu), v) + a(y^k(\mu), v; \mu) + \int_\Omega g^{\mathrm{nl}}(y^k(\mu); x; \mu)\, v = b(v) y(t^k), \ \forall v \in \mathcal{Y}.$$

Assumptions:

- $g^{\mathrm{nl}} : \mathbb{R} \times \Omega \times \mathcal{D} \to \mathbb{R} \quad$ continuous;
- $g^{\mathrm{nl}}(y_1; x; \mu) \leq g^{\mathrm{nl}}(y_2; x; \mu), \ \forall y_1 \leq y_2;$
- $\forall y \in \mathbb{R}, \ y\, g^{\mathrm{nl}}(y; x; \mu) \geq 0, \ \text{for any } x \in \Omega, \ \mu \in \mathcal{D}.$

Standard RB Approach

Sample Computation:

We expand $y_N(t^k;\mu) = \sum_{j=1}^{N} y_{Nj}(t^k;\mu)\,\zeta_j,$

and obtain $\qquad (v = \zeta_i,\ \ i,j \in \mathcal{N})$

$$\Omega g(y_N(t^k;\mu);x;\mu)\zeta_i =$$

$$\int_\Omega g\left(\sum_{j=1}^{N} y_{Nj}(t^k;\mu)\,\zeta_j; x; \mu\right)\zeta_i$$

$\Rightarrow \mathcal{N}$-dependent online cost.

Note

- Standard RB-Galerkin recipe suffices for (at most) quadratic nonlinearities: $\mathcal{O}(N^4)$ online cost ([VPP03, VP05, NVP05]...)
- Higher order or nonpolynomial nonlinearities $\Rightarrow$ EIM

Empirical Interpolation Method

Interpolation Points and Spaces :

$$\begin{aligned} T_M^g &= \{x_1^T \in \Omega, \ldots, x_M^T \in \Omega\} \quad \textit{and} \\ W_M^g &= \mathrm{span}\{\xi_m,\ 1 \leq m \leq M\} \\ &= \mathrm{span}\{q_1, \ldots, q_M\}, \quad 1 \leq M \leq M_{\max}, \end{aligned}$$

ξ_m are chosen by $\mathrm{POD_t} - \mathrm{Greedy}_\mu$ procedure.

Approximation : for given $w^k(\mu) \in Y$

$$g^{\mathrm{nl}}(w^k(\mu); x; \mu) \approx g_M^{\mathrm{nl}, w^k}(x; \mu) = \sum_{m=1}^{M} \varphi_{Mm}^k(\mu)\, q_m(x),$$

where

$$\sum_{m=1}^{M} q_m(x_n^T)\, \varphi_{Mm}^k(\mu) = g^{\mathrm{nl}}(w(x_n^T, t^k; \mu); x_n^T; \mu),\ 1 \leq n \leq M.$$

Note: $\varphi_{Mm}^k(\mu) = \varphi_{Mm}(t^k; \mu)$ function of (discrete) time t^k.

Galerkin Projection

Given $\mu \in \mathcal{D}$, evaluate $\qquad \forall k \in \mathbb{K}$

$$s^k_{N,M}(\mu) = \ell(y^k_{N,M}(\mu))$$

where $y^k_{N,M}(\mu) \in W^y_N$, $1 \le k \le K$, satisfies $\quad y^0_{N,M}(\mu) = 0$

$$\frac{1}{\Delta t} m(y^k_{N,M}(\mu) - y^{k-1}_{N,M}(\mu), v) + a(y^k_{N,M}(\mu), v; \mu)$$

$$+ \int_\Omega g_M^{\mathrm{nl}, y^k_{N,M}}(x;\mu)\ v = b(v)\ y(t^k), \quad \forall\, v \in W^y_N.$$

Computational Procedure:

- Admits an *offline-online* treatment
- *Online cost*† is $\mathcal{O}(MN^2 + N^3)$ and thus independent of $\mathcal{N}$.

†Cost per Newton iteration per timestep.

Energy Norm & Output Bound

Energy norm bound [Gre12a]

$$\Delta_{N,M}^{y\,k}(\mu) = \left\{ \frac{2\Delta t}{\alpha_{\mathrm{LB}}(\mu)} \left(\underbrace{\sum_{k'=1}^{k} \varepsilon_{N,M}^{k'}(\mu)^2}_{\text{linear}} + \underbrace{\vartheta_M^{q\;2} \sum_{k'=1}^{k} \hat{\varepsilon}_M^{k'}(\mu)^2}_{\text{nonlinear}} \right) \right\}^{\frac{1}{2}},$$

contribution to error bound

where

$\alpha_{\mathrm{LB}}(\mu)$ … Lower bound of "a" - coercivity constant,

$\varepsilon_{N,M}^{k}(\mu)$ … dual norm of residual,

$\hat{\varepsilon}_M^{k}(\mu)$ … interpolation induced error.

Output bound

$$\Delta_{N,M}^{s}(t^k;\mu) \equiv \left(\sup_{v \in Y} \frac{\ell(v)}{\|v\|_{L^2(\Omega)}} \right) \Delta_{N,M}^{y\,k}(\mu).$$

Model Problem

Given $\mu = (\mu_1, \mu_2) \in \mathcal{D} \equiv [0.01, 10]^2$, evaluate $\qquad \Omega =]0,1[^2$

$$s^k(\mu) = \int_\Omega y^k_{N,M}(\mu)$$

where $y^k_{N,M}(\mu) \in Y,\ 1 \leq k \leq K$, satisfies $\ y^0(\mu) = 0$

$$\frac{1}{\Delta t} m(y^k_{N,M}(\mu) - y^{k-1}_{N,M}(\mu), v) + a(y^k_{N,M}(\mu), v)$$

$$+ \int_\Omega g^{\mathrm{nl}}(y^k(\mu); x; \mu)\, v = b(v)\, \sin(2\pi t^k), \quad \forall\, v \in Y,$$

with $g^{\mathrm{nl}}(y^k(\mu); x; \mu) = \mu_1 \dfrac{e^{\mu_2\, y^k(\mu)} - 1}{\mu_2}$.

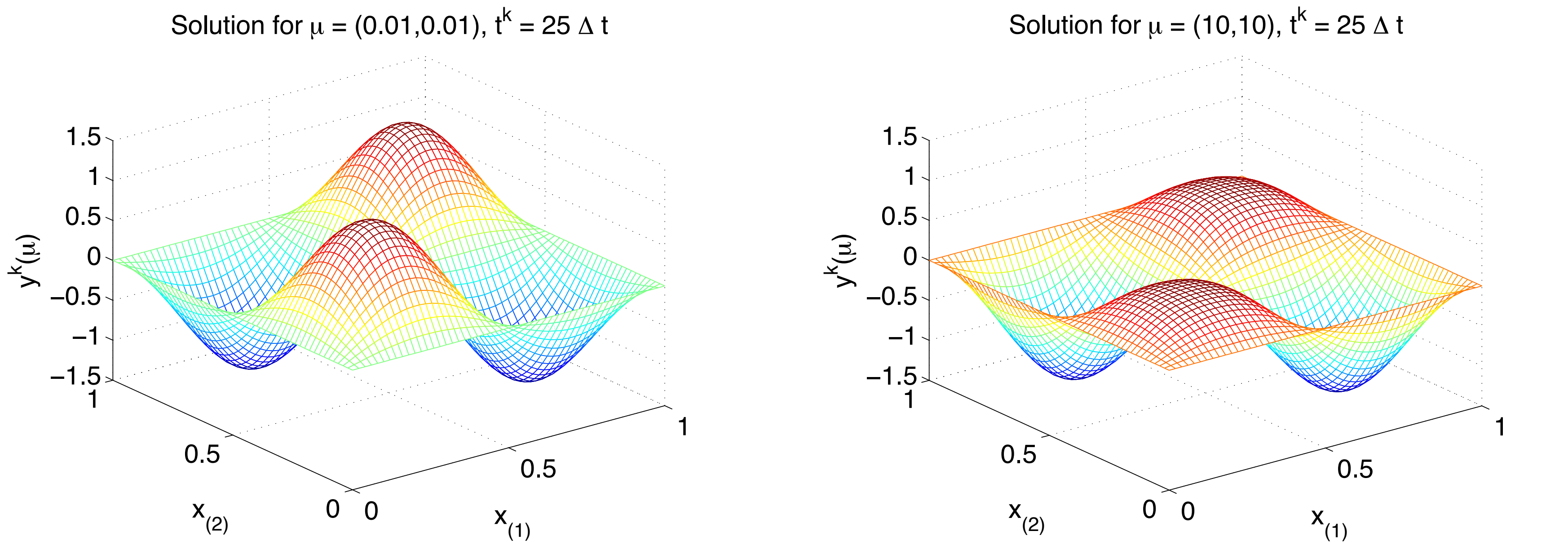
Truth Approximation

- Space: $Y \subset Y^{\mathrm{e}} \equiv H^1_0(\Omega)$ with dimension $\mathcal{N} = 2601$;
- Time: $\bar{I} = (0, 2],\ \Delta t = 0.01$, and thus $K = 200$.

Sample Results

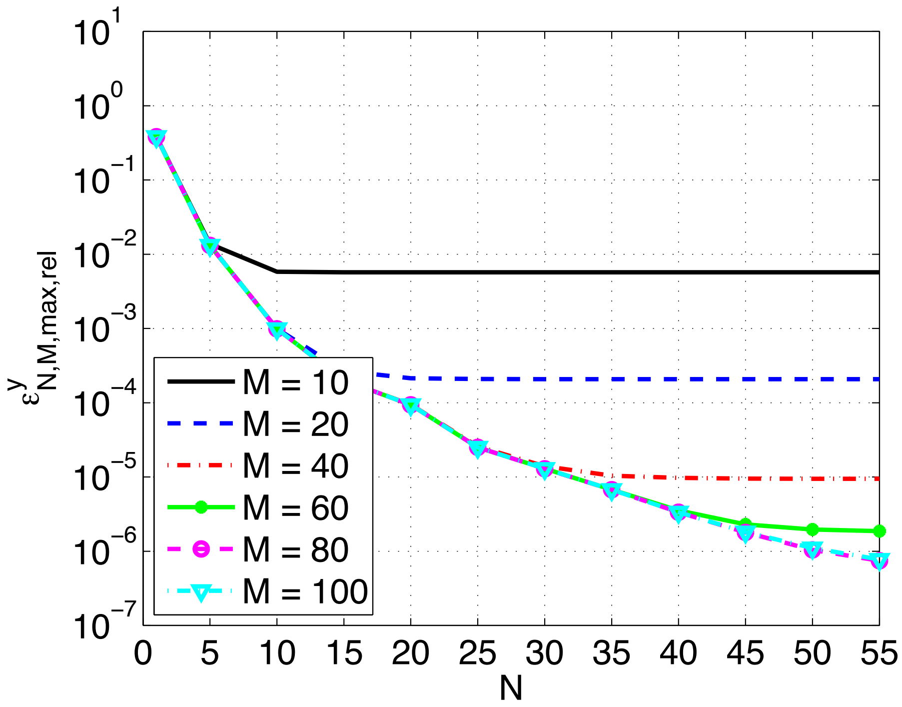
Truth solution $y(t^k;\mu)$ at time $t^k = 25\Delta t$ and

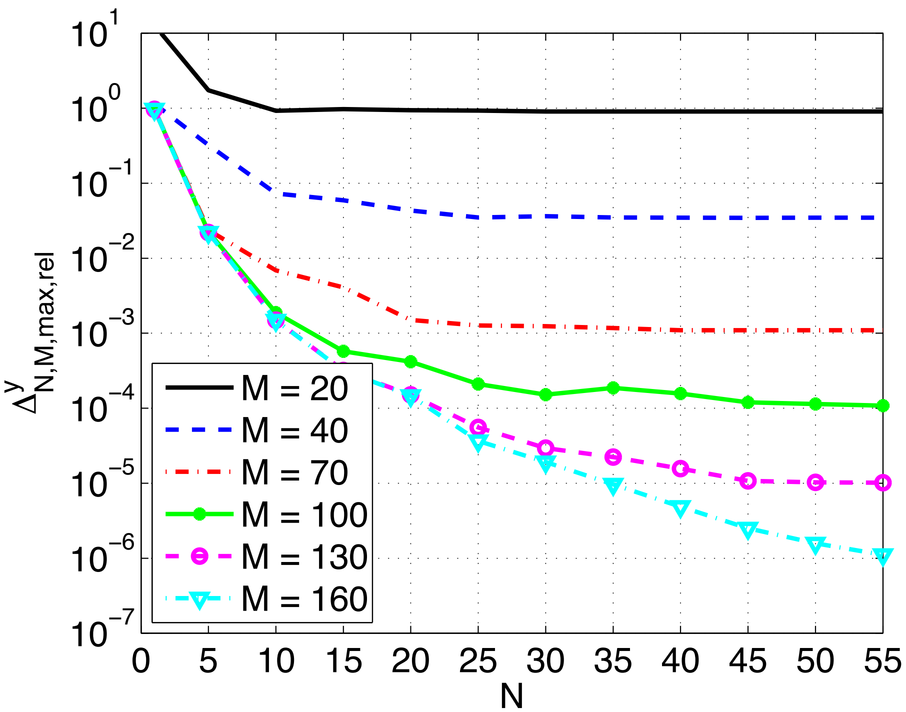
$$\mu = (0.01, 0.01) \qquad\qquad \mu = (10, 10)$$



$$b(v) = 100 \int_\Omega v \, \sin(2\pi x_1) \cos(2\pi x_2)$$

Convergence: Energy Norm





Results for random sample $\Xi_{\mathbf{test}} \in \mathcal{D}$ of size 225.

- “Plateau” in curves for M fixed.
- “Knees” reflect balanced contribution of both error terms.
- Sharp bounds require conservative choice of M.

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Introduction to Reduced Basis Methods: Theory and Applications

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PART II

Overview

Part I: Introduction to the Reduced Basis Method

- Motivation
- RB for the Simplest Case
- Generalizations
  - EIM for Non-Affine and Nonlinear Problems

Part II: RB + Data Assimilation

Part III: Applications + Exercises (James Nichols)

Overview

Part I: Introduction to the Reduced Basis Method

Part II: RB + Data Assimilation

Generalized EIM

Parametrized Background Data Weak Method (PBDW)

(Optimal Control)

4DVAR - Data Assimilation

3DVAR - Data Assimilation + Sensor Placement

Part III: Applications + Exercises (James Nichols)

EIM Greedy Approach

We then proceed by induction to generate S_M^g, W_M^g, and T_M:

For $1 \leq M \leq M_{\max}$, we first solve the interpolation problem

$$g_M(\boldsymbol{x}_i;\mu) = \sum_{j=1}^{M} B_{ij}^M \varphi_{M\,j}(\mu) = g(\boldsymbol{x}_i;\mu), \quad 1 \leq i \leq M,$$

where $B_{ij}^M = q_j(\boldsymbol{x}_i), 1 \leq i,j \leq M$, then compute

$$g_M(\boldsymbol{x};\mu) \equiv \sum_{m=1}^{M} \varphi_{M\,m}(\mu) q_m(\boldsymbol{x}),$$

and evaluate the interpolation error

$$\varepsilon_M(\mu) = \|g(\cdot;\mu) - g_M(\cdot;\mu)\|_{L^\infty(\Omega)}$$

for all $\mu \in \Xi_{\text{train}}^g$.

EIM Greedy Approach

We then determine

$$\mu^g_{M+1} \equiv \arg \max_{\mu \in \Xi^g_{\mathrm{train}}} \varepsilon_M(\mu)$$

and compute $\xi_{M+1} \equiv g(x; \mu^g_{M+1})$.

To generate the interpolation points we solve the linear system

$$\sum_{j=1}^{M} \sigma_j^M \, q_j(x_i) = \xi_{M+1}(x_i), \quad 1 \leq i \leq M$$

and we set $r_{M+1}(x) = \xi_{M+1}(x) - \sum_{j=1}^{M} \sigma_j^M \, q_j(x)$.

The next interpolation point is

$$x_{M+1} = \arg \max_{x \in \Omega} |r_{M+1}(x)|$$

and $q_{M+1}(x) = r_{M+1}(x)/r_{M+1}(x_{M+1})$.

GEIM

Function space interpolation

Approximate the function

$$\varphi \in F$$

A set of functions, e.g. solutions from different models with different parameters

with its interpolation

$$\mathcal{I}_M[\varphi] := \sum_{i=1}^{M} \tilde{\alpha}_j^M(\varphi)\tilde{q}_j$$

Interpolation functions

Interpolation coefficients

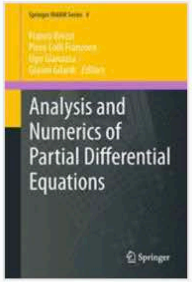
where the coefficients $\tilde{\alpha}_j^M(\varphi)$ are chosen such that

$$\sigma_i(\mathcal{I}_M[\varphi]) := \sigma_i(\varphi)$$

Linear functionals

Data, e.g., measurements

GEIM



Analysis and Numerics of Partial Differential Equations pp 221-235 | Cite as

A Generalized Empirical Interpolation Method: Application of Reduced Basis Techniques to Data Assimilation

Authors | Authors and affiliations

Yvon Maday, Olga Mula

- How can we choose the measurement functionals from a library?
- How can we choose the interpolating functions?
- What about well-posedness of this formulation?
- …

GEIM

State Estimation

Given measurement data $d_i = \sigma_i(y_{\text{true}})$ of some unknown state y_{true}

Assume y_{true} can be expected to be close to a set F of candidate states

Approximate y_{true} using

$$y_{\text{true}} \approx \sum_{i=1}^{M} \tilde{\alpha}_j^M(\varphi)\tilde{q}_j \qquad \text{where} \qquad d_i = \sum_{j=1}^{M} \tilde{\sigma}_j^M \sigma_i(\tilde{q}_j), \quad \forall\ i = 1, \ldots, M$$

This corresponds to:

$$y \in \operatorname{span}\{\ \tilde{q}_i,\ i = 1, \ldots, M\ \} \quad \text{such that} \quad \sigma_i(y) = d_i, \quad i = 1, \ldots, M$$

GEIM

Initialization

$$\tilde{\varphi}_1 := \arg\max_{\phi \in F} ||\varphi||$$

Generating function

$$\sigma_1 := \arg\max_{\sigma \in \Sigma} |\sigma(\varphi_1)|$$

First measurement functional

$$\tilde{q}_1 := \frac{\tilde{\varphi}_1}{\sigma_1(\tilde{\varphi}_1)}$$

First interpolating basis function

GEIM

Iterative Procedure

Suppose $\{\tilde{q}_1, \ldots, \tilde{q}_{M-1}\}$ and $\{\sigma_1, \ldots, \sigma_{M-1}\}$ have been constructed.

$$\tilde{\varphi}_M := \arg\max_{\phi \in F} ||\varphi - \mathcal{I}_{M-1}[\varphi]||$$

Function that is currently approximated the worst

$$\sigma_M := \arg\sup_{\sigma \in \Sigma} |\sigma(\varphi_M - \mathcal{I}_{M-1}[\varphi])|$$

Next measurement functional

$$\tilde{q}_M := \frac{\tilde{\varphi}_M - \mathcal{I}_{M-1}[\varphi]}{\sigma_1(\tilde{\varphi}_M - \mathcal{I}_{M-1}[\varphi])}$$

Next interpolation function

PBDW

Unlimited-observations PBDW statement

Find $y_N^* \in \mathcal{Y},\ z_N^* \in \mathcal{Z}_N,\ \eta_N^* \in \mathcal{Y} \quad \text{s.t.}$

$$(y_N^*, z_N^*, \eta_N^*) = \arg \inf_{\substack{y_N \in \mathcal{Y} \\ z_N \in \mathcal{Z}_N \\ \eta_N \in \mathcal{Y}}} \|\eta_N\|^2$$

Subject to

$$(y_N, v) = (\eta_N, v) + (z_N, v) \quad \forall v \in \mathcal{Y},$$

$$(y_N, \phi) = (y^{\text{true}}, \phi) \quad \forall \phi \in \mathcal{Y}.$$

PBDW

Unlimited-observations PBDW statement

Introduce library of observation functionals

$$\mathcal{L} = \{\ell \in \mathcal{Y}' \mid \ell = \ell_m^o\}$$

where (for example) $\ell_m^\circ(v) = \text{Gauss}\,(v; x_m^c, r_m)$

Let $\mathcal{T}_M = \text{span}\,\{R_\mathcal{Y}\, \ell_m^\circ\}_{m=1}^M\,, \quad M = 1, \ldots, M_{\max}, \ldots$

where $(v,\ R_\mathcal{Y}\, \ell_m^\circ) = \ell_m^\circ(v) \quad \forall v \in \mathcal{Y}$

PBDW

Limited-observations PBDW statement

Find $(y^*_{N,M} \in \mathcal{Y},\ z^*_{N,M} \in \mathcal{Z}_N,\ \eta^*_{N,M} \in \mathcal{Y})$

$$(y^*_{N,M},\ z^*_{N,M},\ \eta^*_{N,M}) = \arg \inf_{\substack{y_{N,M} \in \mathcal{Y} \\ z_{N,M} \in \mathcal{Z}_N \\ \eta_{N,M} \in \mathcal{Y}}} \|\eta_{N,M}\|^2$$

subject to

$$(y_{N,M}, v) = (\eta_{N,M}, v) + (z_{N,M}, v) \quad \forall v \in \mathcal{Y},$$

$$(y_{N,M}, \phi) = (y^{\text{true}}, \phi) \quad \forall \phi \in \mathcal{T}_M.$$

Unlimited-observations PBDW statement

The PBDW approximation error satisfies

$$\left\|\eta_N^* - \eta_{N,M}^*\right\| \leqslant \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

$$\left\|z_N^* - z_{N,M}^*\right\| \leqslant \frac{1}{\beta_{N,M}} \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

$$\left\|y^{\text{true}} - y_{N,M}^*\right\| \leqslant \left(1 + \frac{1}{\beta_{N,M}}\right) \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

where the stability constant $\beta_{N,M}$ is defined by

$$\beta_{N,M} \equiv \inf_{z \in \mathcal{Z}_N} \sup_{q \in \mathcal{T}_M} \frac{(z, q)}{\|z\| \|q\|}.$$

PBDW

Unlimited-observations PBDW statement

The PBDW approximation error satisfies

$$\left\|\eta_N^* - \eta_{N,M}^*\right\| \leqslant \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{ true }} - z - q\right\|,$$

$$\left\|z_N^* - z_{N,M}^*\right\| \leqslant \frac{1}{\beta_{N,M}} \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

$$\left\|y^{\text{ true }} - y_{N,M}^*\right\| \leqslant \left(1 + \frac{1}{\beta_{N,M}}\right) \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{ true }} - z - q\right\|,$$

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PBDW

Unlimited-observations PBDW statement

The PBDW approximation error satisfies

$$\left\|\eta_N^* - \eta_{N,M}^*\right\| \leqslant \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

$$\left\|z_N^* - z_{N,M}^*\right\| \leqslant \frac{1}{\beta_{N,M}} \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

$$\left\|y^{\text{true}} - y_{N,M}^*\right\| \leqslant \left(1 + \frac{1}{\beta_{N,M}}\right) \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

where the stability constant $\beta_{N,M}$ is defined by

$$\beta_{N,M} \equiv \inf_{z \in \mathcal{Z}_N} \sup_{q \in \mathcal{T}_M} \frac{(z, q)}{\|z\| \|q\|}.$$

PBDW

Unlimited-observations PBDW statement

The PBDW approximation error satisfies

$$\left\| \eta_N^* - \eta_{N,M}^* \right\| \leqslant \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\| y^{\text{true}} - z - q \right\|,$$

$$\left\| z_N^* - z_{N,M}^* \right\| \leqslant \frac{1}{\beta_{N,M}} \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\| y^{\text{true}} - z - q \right\|,$$

$$\left\| y^{\text{true}} - y_{N,M}^* \right\| \leqslant \left(1 + \frac{1}{\beta_{N,M}} \right) \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\| y^{\text{true}} - z - q \right\|,$$

where the stability constant $\beta_{N,M}$ is defined by

$$\beta_{N,M} \equiv \inf_{z \in \mathcal{Z}_N} \sup_{q \in \mathcal{T}_M} \frac{(z, q)}{\|z\| \|q\|}.$$

PBDW

Unlimited-observations PBDW statement

The PBDW approximation error satisfies

$$\left\|\eta_N^* - \eta_{N,M}^*\right\| \leqslant \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

$$\left\|z_N^* - z_{N,M}^*\right\| \leqslant \frac{1}{\beta_{N,M}} \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

$$\left\|y^{\text{true}} - y_{N,M}^*\right\| \leqslant \left(1 + \frac{1}{\beta_{N,M}}\right) \inf_{q \in \mathcal{T}_M \cap \mathcal{Z}_N^\perp} \inf_{z \in \mathcal{Z}_N} \left\|y^{\text{true}} - z - q\right\|,$$

where the stability constant $\beta_{N,M}$ is defined by

$$\beta_{N,M} \equiv \inf_{z \in \mathcal{Z}_N} \sup_{q \in \mathcal{T}_M} \frac{(z,q)}{\|z\|\|q\|}.$$

Optimal Control

with

M. Kärcher and M. Grepl

Optimal Control

Problem Formulation

$$\min_{u \in U} J(y,u) = \frac{1}{2}\|y - y_d\|^2_{L^2(D)} + \frac{\tau}{2}\|u\|^2_U$$

$$\text{s.t.} \quad \langle Ay, v\rangle = \langle Cu, v\rangle + \langle f, v\rangle, \quad \forall v \in Y,$$

Desired state	$y_d(x), \ x \in \Omega$
Distributed control	$u(x), \ x \in \Omega$
PDE-constraint	state y is governed by a μ-PDE

Optimal Control

Reduced Basis Approximation

$$\min_{u_n \in U_n} J(y_n, u_n) = \frac{1}{2}\|y_n - y_d\|^2_{L^2(D)} + \frac{\tau}{2}\|u_n\|^2_U$$
$$\text{s.t.} \quad \langle A_n y_n, v\rangle = \langle C_n u_n, v\rangle + \langle f_n, v\rangle, \quad \forall v \in Y_n,$$

RB approximation as surrogate $\quad y_n, \; u_n$

Error estimation $\quad \|u^{\mathrm{o}} - u_n^{\mathrm{o}}\|_U \leq \Delta_n^u$

$$|J(u^{\mathrm{o}}) - J(u_n^{\mathrm{o}})| \leq \Delta_n^J$$

Optimal Control

Status

- Order Reduction for

  - sharp (POD) error bounds, but requires FE-solves

    [TRÖLTZSCH & VOLKWEIN, 2009]

  - online-efficient but non-rigorous error estimates

    [DEDÈ, 2010a], [DEDÈ, 2012]

  - online-efficient, rigorous error bounds

    [GREPL & KÄRCHER, 2011], [KÄRCHER & GREPL, 2014]

Optimal Control

Status: Distributed optimal control

- **Perturbation Bound** in [KÄRCHER, 2011]
  - based on [TV09], [GK11], [KG14]
  - online-efficient, separate error bounds for state, control, and adjoint

$$\|u^{\mathrm{o}} - u_m^{\mathrm{o}}\|_U \leq \quad \Delta_n^u = \frac{1}{\tau}\|\tau(u_m^{\mathrm{o}} - u_d) - B^* p_n^{\mathrm{o}}\|_U + \frac{1}{\tau}\gamma_c \Delta_n^p$$

$$\|p^{\mathrm{o}} - p_n^{\mathrm{o}}\|_Y \leq \quad \Delta_n^p \equiv \frac{1}{\alpha_a}\left(\|r_p\|_{Y'} + C_D^2 \Delta_n^y\right)$$

$$\|y^{\mathrm{o}} - y_n^{\mathrm{o}}\|_Y \leq \quad \Delta_n^y \equiv \frac{1}{\alpha_a}\|r_y\|_{Y'}$$

  - depends only on α_a, γ_c, and C_D
  - bound for error in u contains terms which scale as

$$\sim \frac{1}{\tau}\|r_y\|_{Y'}$$

Optimal Control

Status: Distributed optimal control

- **BNB Bound** in [NEGRI, ROZZA, MANZONI & QUARTERONI, 2013]
  - based on the Banach-Nečas-Babuška Theorem and RB for general non-coercive problems
  - consider the entire optimality system

$$\begin{bmatrix} \underline{M} & \underline{0} & \underline{A} \\ \underline{0} & \tau \underline{D} & -\underline{C}^T \\ \underline{A} & -\underline{C} & \underline{0} \end{bmatrix} \begin{bmatrix} \underline{y}^{\mathrm{o}} \\ \underline{u}^{\mathrm{o}} \\ \underline{p}^{\mathrm{o}} \end{bmatrix} = \begin{bmatrix} \underline{M} \\ \tau \underline{D} \\ \underline{0} \end{bmatrix}$$

    and introduce $x = (y, u, p) \in \mathcal{Z}$ to obtain

$$\|x^{\mathrm{o}} - x_n^{\mathrm{o}}\|_{\mathcal{Z}} \leq \frac{1}{\beta_{\mathrm{Ba}}} \|r_x\|_{\mathcal{Z}'}$$

  - online-efficient error bounds, but depends on β_{Ba}
  - provides only combined bounds for state, control, adjoint

Optimal Control

Motivation

- Analyze the optimal control problem as a saddle point problem
- Saddle point results not directly applicable:
  - "A-block" is coercive only on kernel of the "B-block"
  - online-efficient, rigorous error bounds on (y, u)
- But perhaps we can use some elements of the proof …

Optimal Control

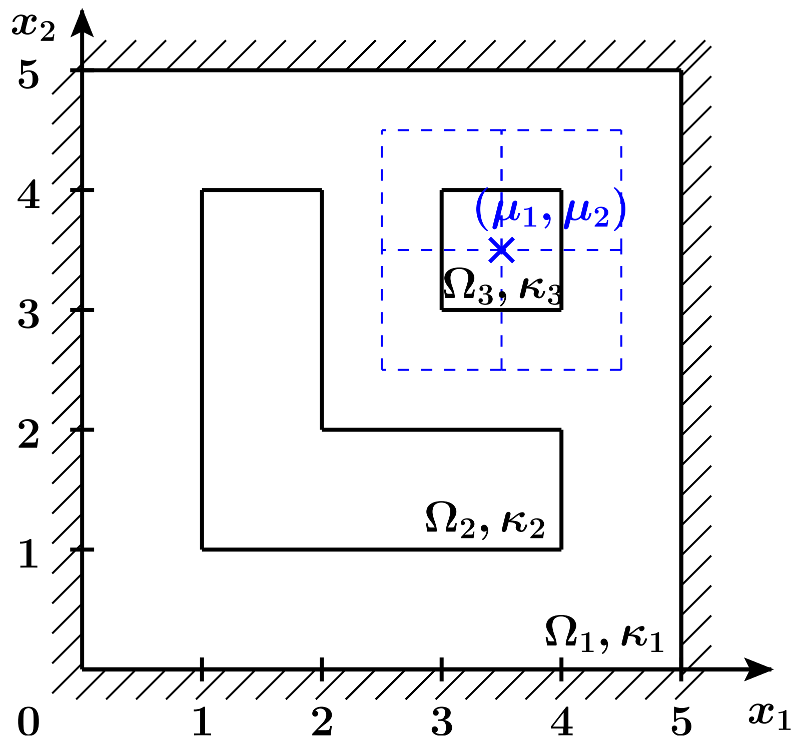
- **Alternative Bound** in [KÄRCHER, GREPL & VEROY, 2014 (preprint)]
  - by direct manipulation of the error residual equations, we obtain

$$\|u^{\mathrm{o}} - u_m^{\mathrm{o}}\|_U \leq \frac{1}{2\tau}\left(\|r_u\|_{U'} + \frac{\gamma_c}{\alpha_a}\|r_p\|_{\mathcal{Y}'}\right) + \frac{1}{2\tau}\left[\left(\|r_u\|_{U'} + \frac{\gamma_c}{\alpha_a}\|r_p\|_{\mathcal{Y}'}\right)^2 + \frac{8\tau}{\alpha_a}\|r_y\|_{\mathcal{Y}'}\|r_p\|_{\mathcal{Y}'} + \frac{\tau C_D^2}{\alpha_a^2}\|r_y\|_{\mathcal{Y}'}^2\right]^{\frac{1}{2}}$$

  - bounds for error in $y_n^{\mathrm{o}},\ p_n^{\mathrm{o}}$ as in perturbation bound
  - online-efficient, separate error bounds for state, control, and adjoint
  - depends only on $\alpha_a, \gamma_c,$ and C_D
  - bound for error in u contains terms which scale as

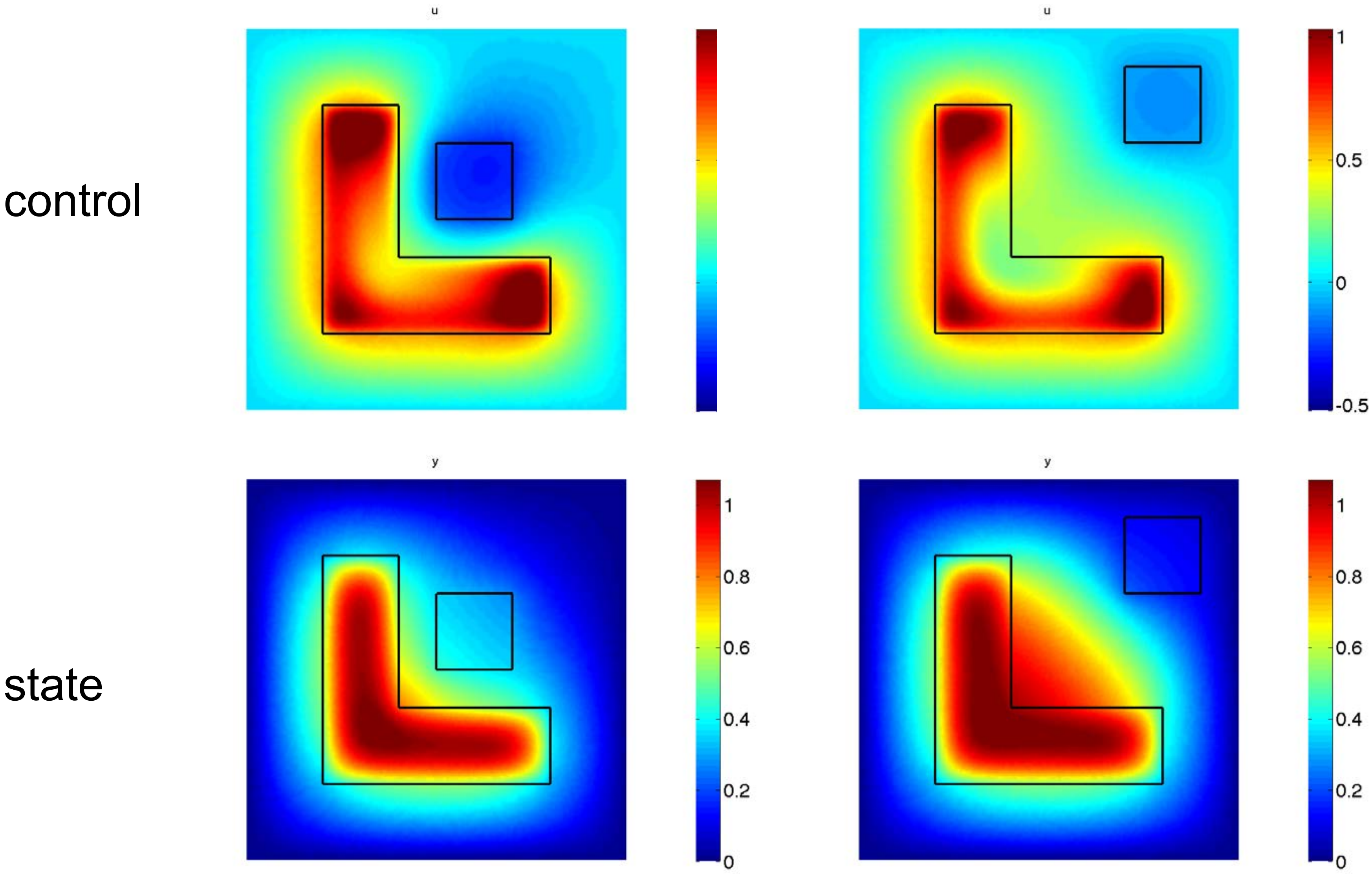
$$\sim \frac{1}{\sqrt{\tau}}\|r_y\|_{\mathcal{Y}'}$$

Model Problem

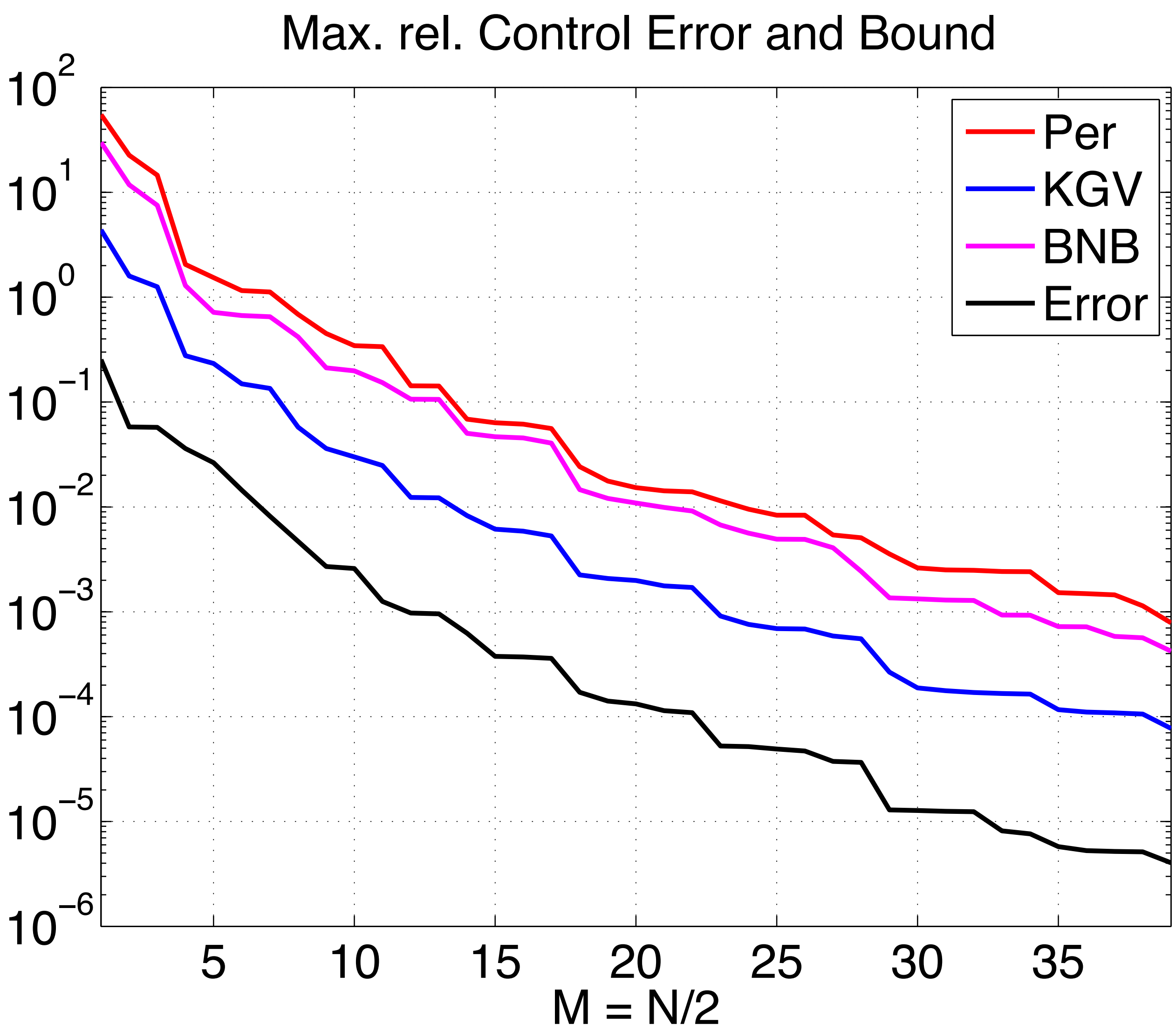


- Steady heat conduction with conductivities $(\kappa_1, \kappa_2, \kappa_3)$
- FE Dimension $\dim(Y) \approx 18,000$
- State $y_d = 1$ in Ω_2 and $y_d = 0$ in Ω_3,
- Regularization parameter: $\tau = 0.1$
- Input parameter: $\mu = (\mu_1, \mu_2) \in \mathcal{D} \equiv [3,4]^2$.

Sample Solutions $(\tau = 0.1)$



Control: Error and Bounds



Timings:

- $t_{\mathrm{FE}} = 1.23s$
- $t_{\mathrm{RB}} \in [1.2, 4.8]\mathrm{ms}$
- $t_{\mathrm{RB},\Delta} \in [2, 7]\mathrm{ms}$

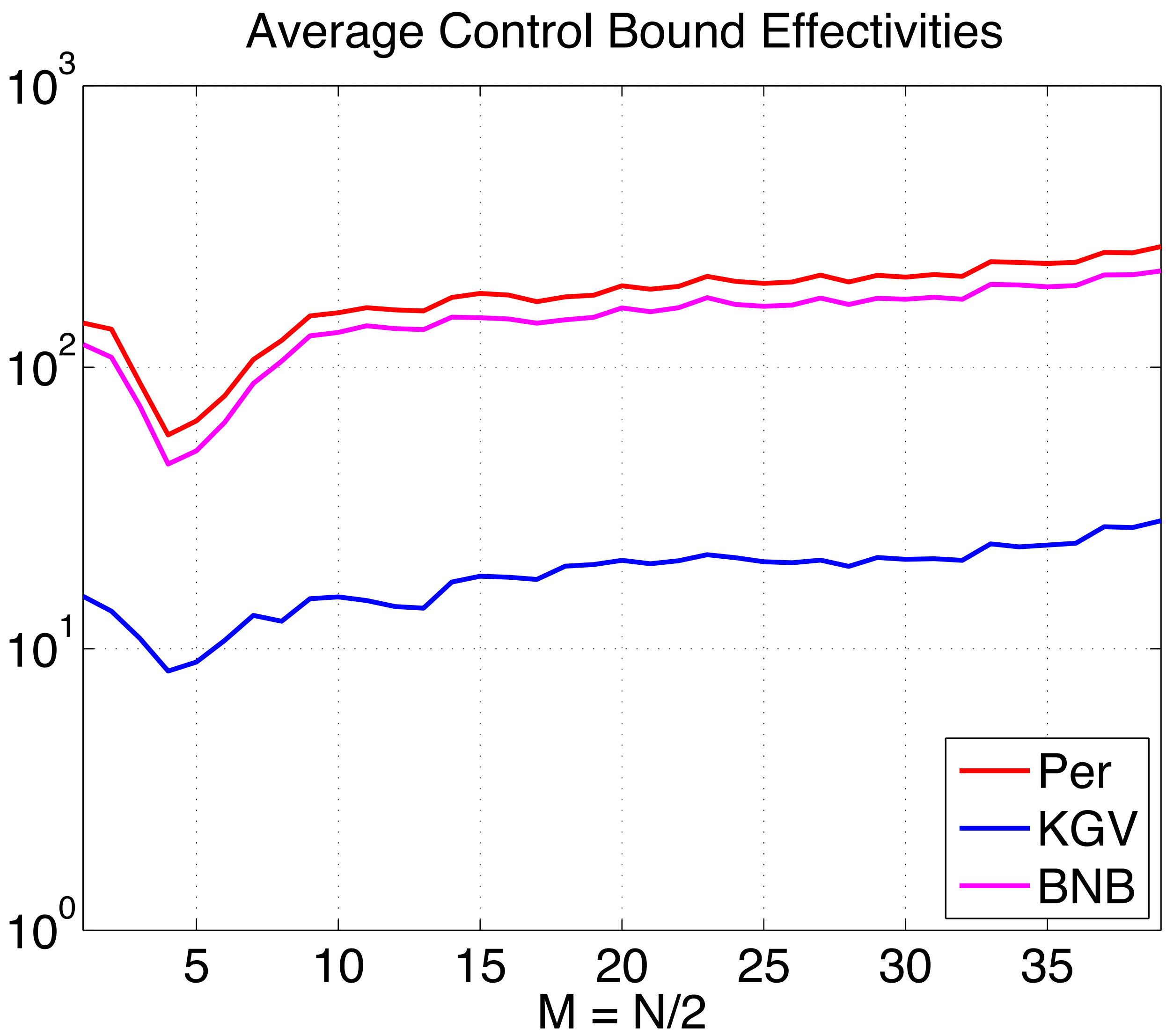
Speedups:

- RB: 256-1025
- RB+Bound: 176-615

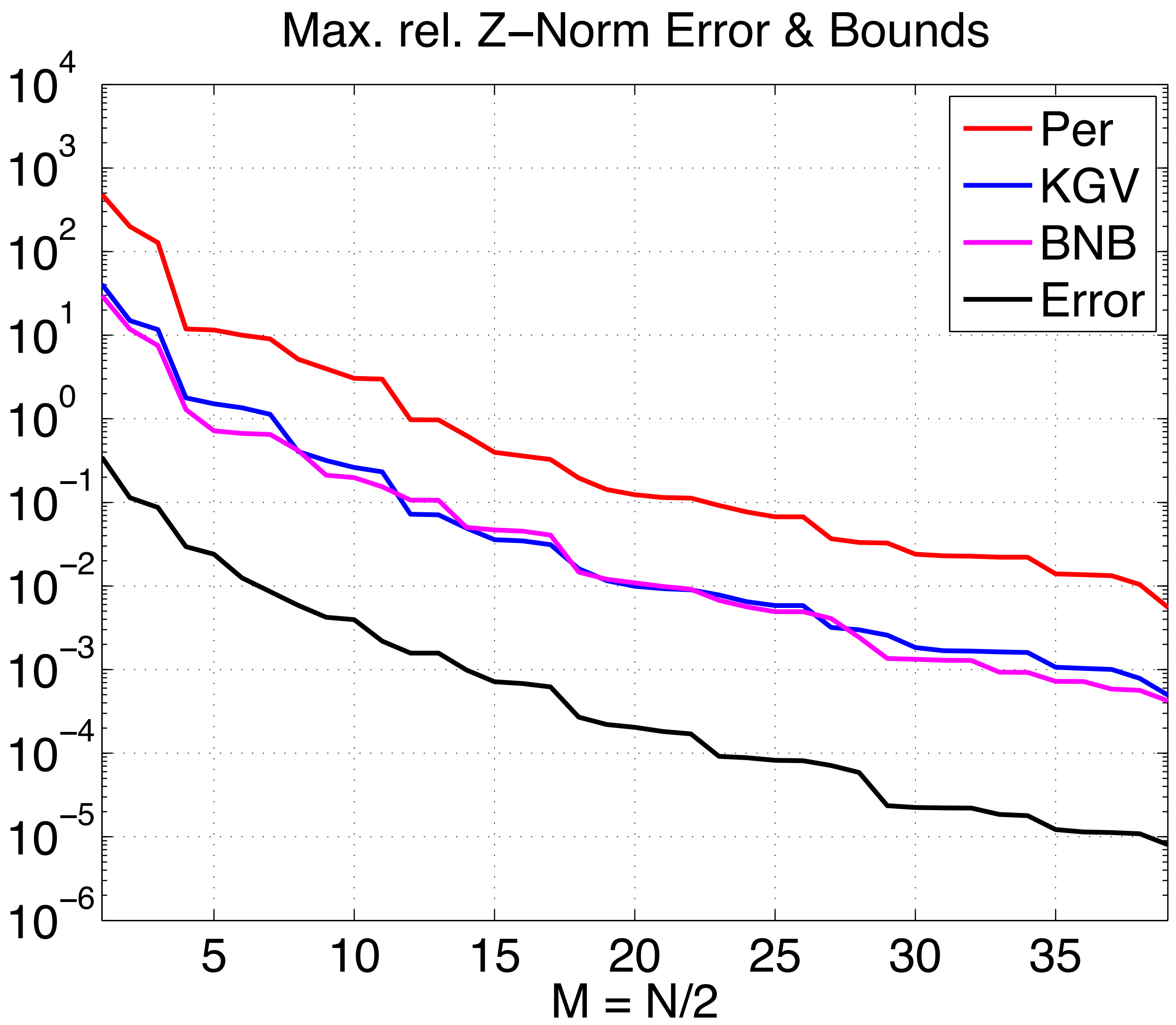
Test set:

- $|\Xi_{\mathrm{test}}| = 20$

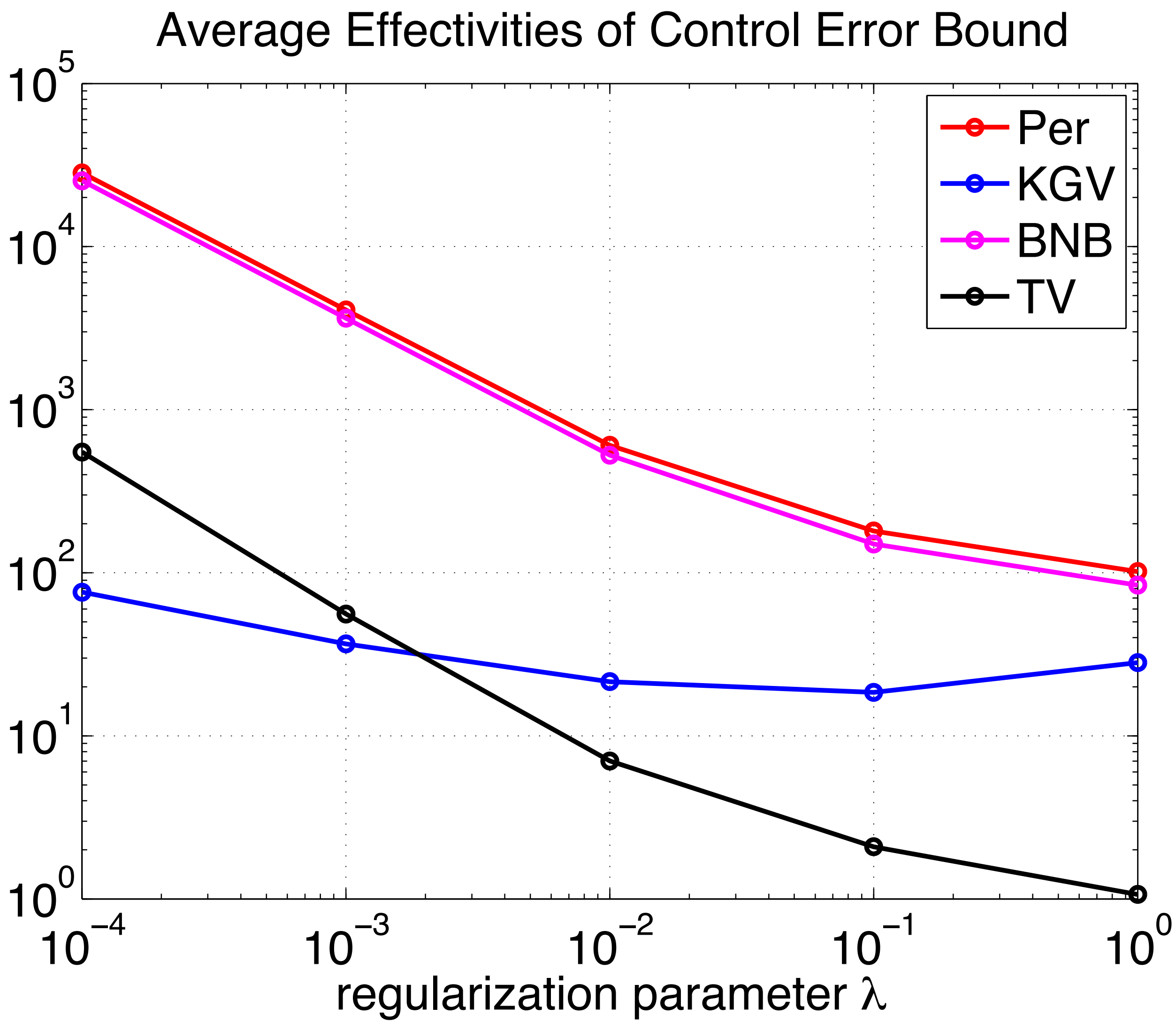
Control: Average Effectivity



Combined Error and Bounds



Effectivities: Influence of τ



Optimal Control (1)

Summary

We developed an **online-efficient** certified reduced basis method for distributed optimal control problems.

The approach provides **separate** bounds for the error in the state, control, and adjoint variables.

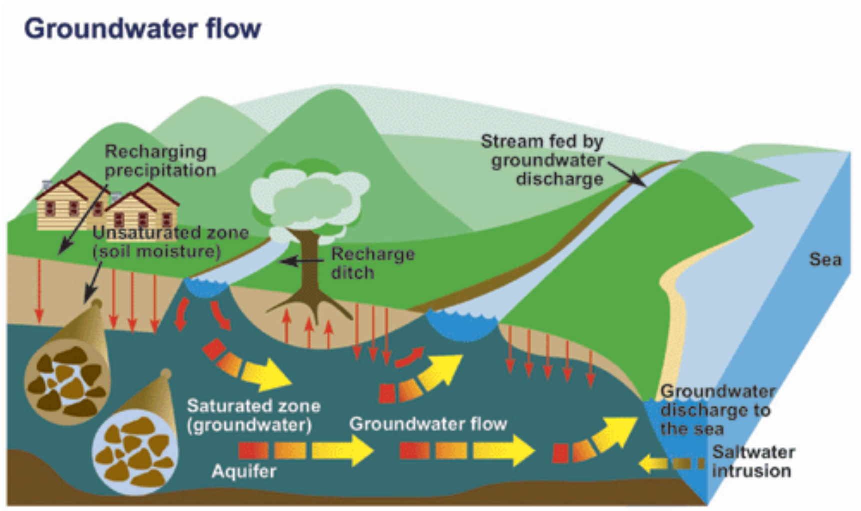
The error bounds are **efficiently computable** and depend only **weakly** on the regularization parameter.

Data Assimilation

with

S. Boyaval, M. Grepl, and M. Kärcher

Motivation - A Geosciences Example



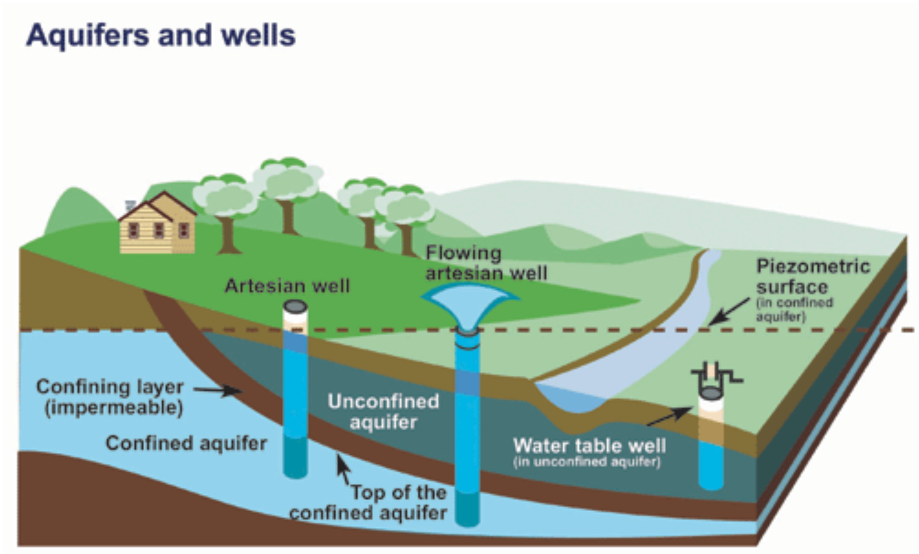
Source: Environment and Climate Canada
`https://www.ec.gc.ca/eau-water`

Groundwater Flow:

- Groundwater management
- Contaminant transport

Goal:

- Predict hydraulic head
- Predict pollutant concentration



Source: Environment and Climate Canada
`https://www.ec.gc.ca/eau-water`

Given:

- Parametrized PDE-model

Issues:

- Parameters unknown
- Model, but possibly erroneous
- Boundary or initial conditions uncertain
- Measurements, possibly noisy

Background

(Variational) Data Assimilation

3D-/4D-VAR [Lorenc '81], [Le Dimet '81], [Courtier '85], …
[Le Dimet & Talagrand '86], … [Navon et al] …

+ Kalman Filter, Bayesian Methods [Law & Stuart '15], [Reich '15], …

MOR + Data Assimilation (+Sensor Placement)

Gappy-POD [Everson & Sirovich '95], [Willcox '06] …

GEIM [Maday & Mula '13] …

PGD (+ EIM) [Nadal, Chinesta, Diez, Fuenmayor & Denia '15] …

PBDW [**Maday, Patera, Penn & Yano '14**, '15], [Taddei '17], [**Maday & Taddei '17(p)**], [Taddei & Patera '18], [Hammond, Chaqir, Bourquin & Maday '18(p)]

OMP [Binev, Cohen, Mula & Nichols '18]

MOR + Optimal Control

RB + OC [Negri, Rozza, Manzoni, Quarteroni '13], [Tröltzsch & Volkwein '09], [**Kärcher, Tokoutsi, Grepl & V. '18**]

4DVAR

4DVAR (μ)

$$\min_{\mu \in \mathcal{D}} \min_{u \in \mathcal{U}} \quad \frac{1}{2}\|u - u_b\|_{\mathcal{U}}^2 \quad + \quad \frac{\lambda}{2}\sum_{k=1}^{K} \Delta t \|C y^k - y_d^k\|_D^2$$

$$\text{s.t.} \quad m(y^k, \nu) = m(y^{k-1}, \nu) - \Delta t \; a(y^k, \nu; \mu) + \Delta t \; f(\nu),$$

$$\forall\, \nu \in Y, \; k = 1, \ldots, K$$

$$y^0 = u$$

Solve for μ^* and the estimate $(u^*(\mu^*), y^*(\mu^*))$.

Optimal Control

Problem Formulation

$$\min_{u \in U} J(y,u) = \frac{1}{2}\|y - y_d\|^2_{L^2(D)} + \frac{\tau}{2}\|u\|^2_U$$
$$\text{s.t.} \quad \langle Ay, v\rangle = \langle Cu, v\rangle + \langle f, v\rangle, \quad \forall v \in Y,$$

Desired state	$y_d(x), \ x \in \Omega$
Distributed control	$u(x), \ x \in \Omega$
PDE-constraint	state y is governed by a μ-PDE

4DVAR

4DVAR (μ)

$$\min_{\mu\in\mathcal{D}}\min_{u\in\mathcal{U}} \quad \frac{1}{2}\|u-u_b\|^2_{\mathcal{U}} \quad + \quad \frac{\lambda}{2}\sum_{k=1}^{K}\Delta t\|Cy^k-y_d^k\|^2_D$$

$$\text{s.t.} \quad m(y^k,\nu) = m(y^{k-1},\nu) - \Delta t\; a(y^k,\nu;\mu) + \Delta t\; f(\nu),$$

$$\forall\, \nu\in Y,\; k=1,\ldots,K$$

$$y^0 = u$$

Solve for $\mu^*$and the estimate $(u^*(\mu^*), y^*(\mu^*))$.

4DVAR

Reduced Order 4DVAR (μ)

$$\min_{\mu \in \mathcal{D}} \min_{u_N \in \mathcal{U}_N} \quad \frac{1}{2} \| u_N - u_b \|_{\mathcal{U}}^2 \quad + \quad \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \| C y_N^k - y_d^k \|_D^2$$

$$\text{s.t.} \quad m(y_N^k, \nu) = m(y_N^{k-1}, \nu) - \Delta t \; a(y_N^k, \nu; \mu) + \Delta t \; f(\nu),$$

$$\forall \, \nu \in Y_N, \; k = 1, \ldots, K$$

$$y_N^0 = u_N$$

Solve for μ^* and the estimate $(u^*(\mu^*), y^*(\mu^*))$.

4DVAR

Reduced Order 4DVAR (μ)

$$\min_{\mu \in \mathcal{D}} \min_{u_N \in \mathcal{U}_N} \frac{1}{2} \|u_N - u_b\|_{\mathcal{U}}^2 + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \|C y_N^k - y_d^k\|_D^2$$

$$\text{s.t.} \quad m(y_N^k, \nu) = m(y_N^{k-1}, \nu) - \Delta t\; a(y_N^k, \nu; \mu) + \Delta t\; f(\nu),$$

$$\forall\, \nu \in Y_N,\; k = 1, \ldots, K$$

$$y_N^0 = u_N$$

Solve for μ^* and the estimate $(u^*(\mu^*), y^*(\mu^*))$.

Order Reduction for

- PDE governing model dynamics
- Optimization space

[Robert, Durbiano, Blayo, Verron, Blum, Le Dimet 2005], [Chen, Navon, Fang 2009], [Dimitriu, Apreutesei, Stefanescu 2010], [Nadal, Chinesta, Diez, Fuenmayor & Denia '15] …

4D-Var (μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u \in \mathcal{U}} \frac{1}{2}\|u(\mu) - u_b\|_{\mathcal{U}}^2 + \frac{\lambda}{2}\sum_{k=1}^{K} \Delta t \|Cy^k(\mu) - y_d^k\|_D^2$$

$$\text{s.t.} \quad m(y^{k+1}, v) = m(y^k, v) - \Delta t a(y^k, v; \mu) + \Delta t f(v), \quad \forall\, v \in Y,\ 1 \leq k \leq K$$

$$y^{\circ} = u$$

for μ^* and the corresponding $(u^*(\mu^*), y^*(\mu^*))$.

Lagrangian

$$\mathcal{L}(y, p, u; \mu) = \frac{1}{2}\|u - u_b\|_{\mathcal{U}}^2 + \frac{\lambda}{2}\sum_{k=1}^{K} \Delta t \|Cy^k - y_d^k\|_D^2 + \sum_{k=1}^{K} m(y^k, p^k) - m(y^{k-1}, p^k) + \Delta t a(y^k, p^k) - \Delta t f(p^k),$$

Reduced Optimality Conditions

$$\begin{aligned} f(\phi) - a(y_N^k, \phi) - \frac{1}{\Delta t} m(y_N^k - y_N^{k-1}, \phi) &= \quad 0 && \mathcal{L}_p \\ \lambda(C y_N^k - y_{\mathrm{d}}^k, C\varphi)_D - \frac{1}{\Delta t} m(\varphi, p_N^k - p_N^{k+1}) + a(\varphi, p_N^k; \mu) &= \quad 0 && \mathcal{L}_y \\ m(\psi, p_N^1) - (u_N - u_{\mathrm{b}}, \psi)_U &= \quad 0 && \mathcal{L}_u \end{aligned}$$

for all $\phi \in Y_N,\ \varphi \in Y_N,\ \psi \in U_N,$ where

CONTROL $\quad U_N = \mathrm{span}\{\ u^*(\mu_i),\ i = 1, \ldots, N\}$

STATE/ADJOINT $\quad Y_N = \mathrm{span}\{\ \mathrm{POD}(y^*(\mu_i)),\ \mathrm{POD}(p^*(\mu_i)),\ i = 1, \ldots, N\}$

4DVAR

Reduced-Order 4DVAR (μ)

Solve $$\min_{\mu \in \mathcal{D}} \min_{u_N \in \mathcal{U}_N} \frac{1}{2} \| u_N - u_b \|^2_{\mathcal{U}} + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \left\| C y_N^k - y_d^k \right\|^2_D$$

$$\text{s.t.} \quad m(y_N^k, \nu) = m(y_N^{k-1}, \nu) - \Delta t \; a(y_N^k, \nu; \mu) + \Delta t \; f(\nu),$$

$$\forall \, \nu \in Y_N, \; k = 1, \dots, K$$

$$y_N^0 = u_N$$

for μ^* and the estimate $(u^*(\mu^*), y^*(\mu^*))$.

Can we quantify the error for a given μ ?

CONTROL $\quad ||u^*(\mu) - u_N^*(\mu)||_{\mathcal{U}} \leq \Delta_N^u(\mu)$

STATE $\quad ||y^*(\mu) - y_N^*(\mu)||_{\mathcal{U}} \leq \Delta_N^y(\mu)$

4D-Var

Reduced Optimality Conditions

$$f(\phi) - a(y_N^k, \phi; \mu) - \frac{1}{\Delta t} m(y_N^k - y_N^{k-1}, \phi) = 0 \quad \mathcal{L}_p$$

$$\lambda(Hy_N^k - y_d^k, H\varphi)_D - \frac{1}{\Delta t} m(\varphi, p_N^k - p_N^{k+1}) + a(\varphi, p_N^k; \mu) = 0 \quad \mathcal{L}_y$$

$$m(\psi, p_N^1) - (u_N - u_b, \psi)_{\mathcal{U}} = 0 \quad \mathcal{L}_u$$

$$\phi \in Y_N, \varphi \in Y_N, \psi \in \mathcal{U}_N$$

4D-Var

Reduced Optimality Conditions

$$f(\phi) - a(y_N^k, \phi; \mu) - \frac{1}{\Delta t} m(y_N^k - y_N^{k-1}, \phi) = 0 \quad \mathcal{L}_p$$

$$\lambda(H y_N^k - y_d^k, H\varphi)_D - \frac{1}{\Delta t} m(\varphi, p_N^k - p_N^{k+1}) + a(\varphi, p_N^k; \mu) = 0 \quad \mathcal{L}_y$$

$$m(\psi, p_N^1) - (u_N - u_b, \psi)_{\mathcal{U}} = 0 \quad \mathcal{L}_u$$

$$\phi \in Y_N, \varphi \in Y_N, \psi \in \mathcal{U}_N$$

CONTROL $\quad \mathcal{U}_N = \text{span}\,\{u^*(\mu_i)),\ i = 1, \ldots, N\}$

STATE/ADJOINT $\quad Y_N = \text{span}\,\{\text{POD}(y^*(\mu_i)), \text{POD}(p^*(\mu_i)), \quad i = 1, \ldots, N\}$

4D-Var

Error

STATE $$e_y^k(\mu) := y^{*k}(\mu) - y_N^{*k}(\mu)$$

ADJOINT $$e_p^k(\mu) := p^{*k}(\mu) - p_N^{*k}(\mu)$$

CONTROL $$e_u^k(\mu) := u^{*k}(\mu) - u_N^{*k}(\mu)$$

4D-Var

Error

STATE $e_y^k(\mu) := y^{*k}(\mu) - y_N^{*k}(\mu)$

ADJOINT $e_p^k(\mu) := p^{*k}(\mu) - p_N^{*k}(\mu)$

CONTROL $e_u^k(\mu) := u^{*k}(\mu) - u_N^{*k}(\mu)$

Error Residual Equations

STATE $r_y^k(\phi;\mu) := a(e_y^k, \phi; \mu) + \dfrac{1}{\Delta t} m(e_y^k - e_y^{k-1}, \phi)$

ADJOINT $r_p^k(\varphi, \mu) := \lambda(He_y^k, H\varphi)_D + \dfrac{1}{\Delta t} m(\varphi, e_p^k - e_p^{k+1}) + a(\varphi, e_p^k; \mu)$

CONTROL $r_u(\mu) := (e_u, \psi)_{\mathcal{U}} - m(\psi, e_p^1)$

A Posteriori Error Estimation

We can show that

$$||u^*(\mu) - u_N^*(\mu)||_{\mathcal{U}} \leq \Delta_N^u(\mu) = c_1(\mu) + \sqrt{c_1(\mu)^2 + c_2(\mu)}$$

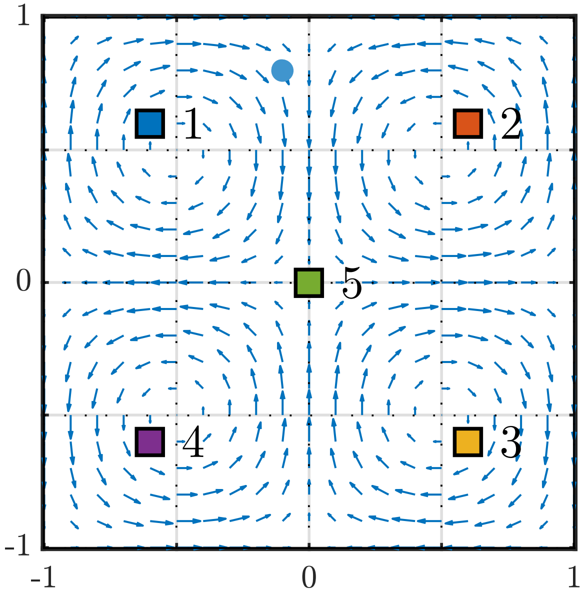
with non-negative terms

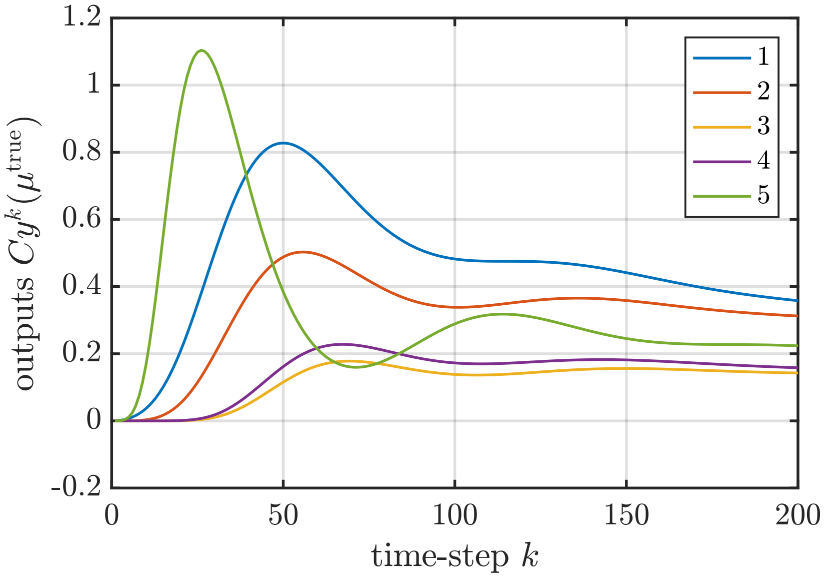
$$c_1 := \frac{1}{2}||r_u||_{\mathcal{U}'} + \frac{1}{\sqrt{\alpha_a^{\mathrm{LB}}}} R_p \qquad c_2 := \left(\frac{1+\sqrt{2}}{\alpha_a^{\mathrm{LB}}} R_y R_p + \frac{\lambda \gamma_C^2}{2(\alpha_a^{\mathrm{LB}})^2} R_y^2 \right)$$

where $R_{y,p} = \left(\tau \sum_{k=1}^{K} ||r_{y,p}^k||_{Y'}^2 \right)^{1/2}$, and r_y^k, r_p^k, r_u are the residuals in the state, adjoint, and control equations.

[Kärcher, Boyaval, Grepl, V., 2018]

Model Problem





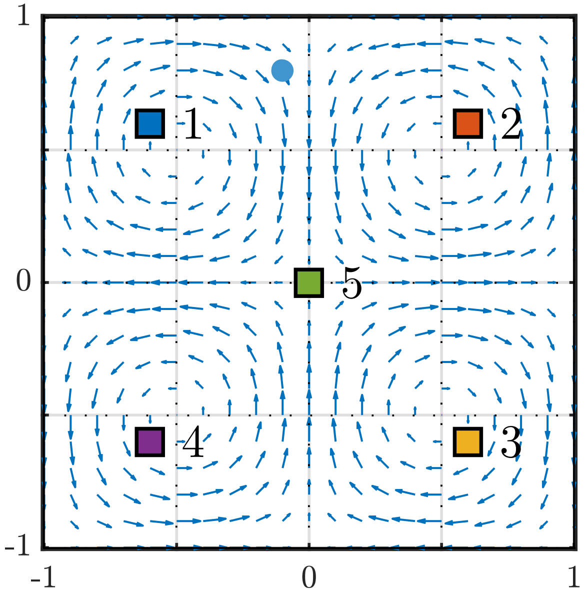
Contaminant transport

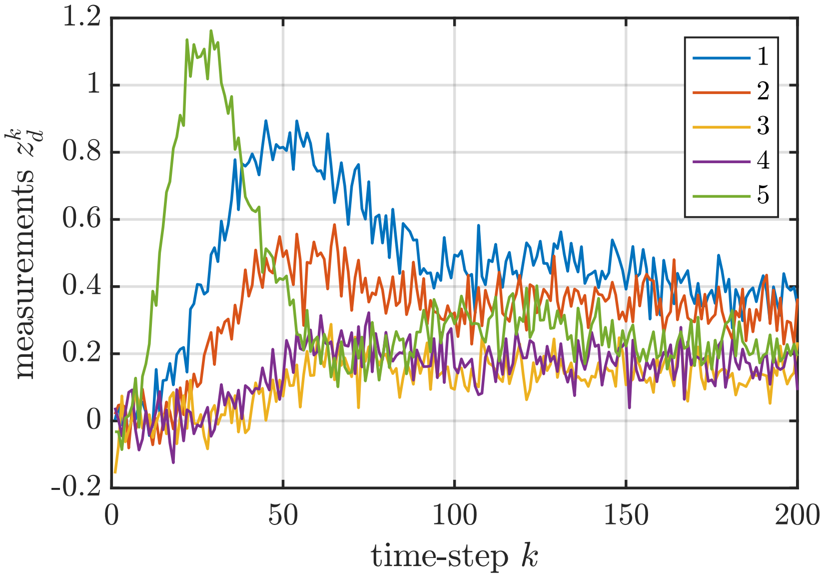
- "Gaussian" initial condition, $\bar{u}_0$
- Known Taylor-Green vortex velocity field
- Parameter $\mu = \mathrm{Pe} \in [10, 50], \bar{\mu} = 30$
- FE dimension $(\mathcal{N} = 13000, K = 200)$

Assumptions:

- Data generated with true initial condition
- Uncertainty due only to noise and "unknown" parameter
- Prior is exact

Model Problem





Contaminant transport

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Assumptions:

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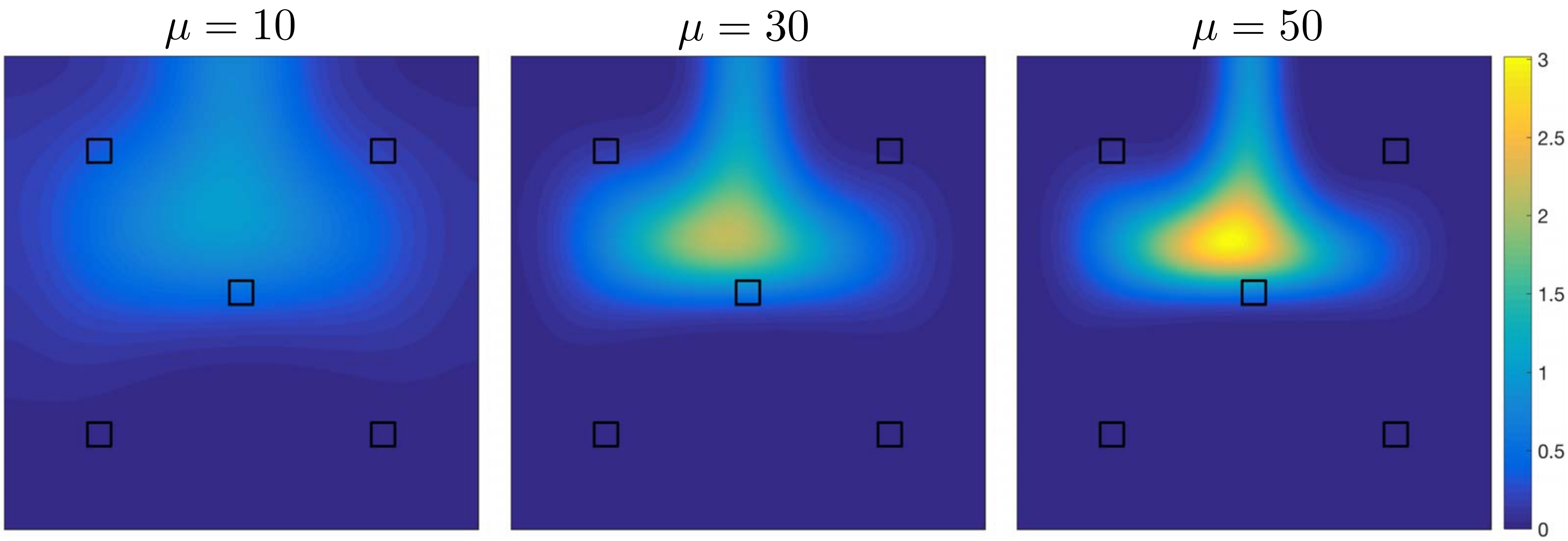
Model Problem

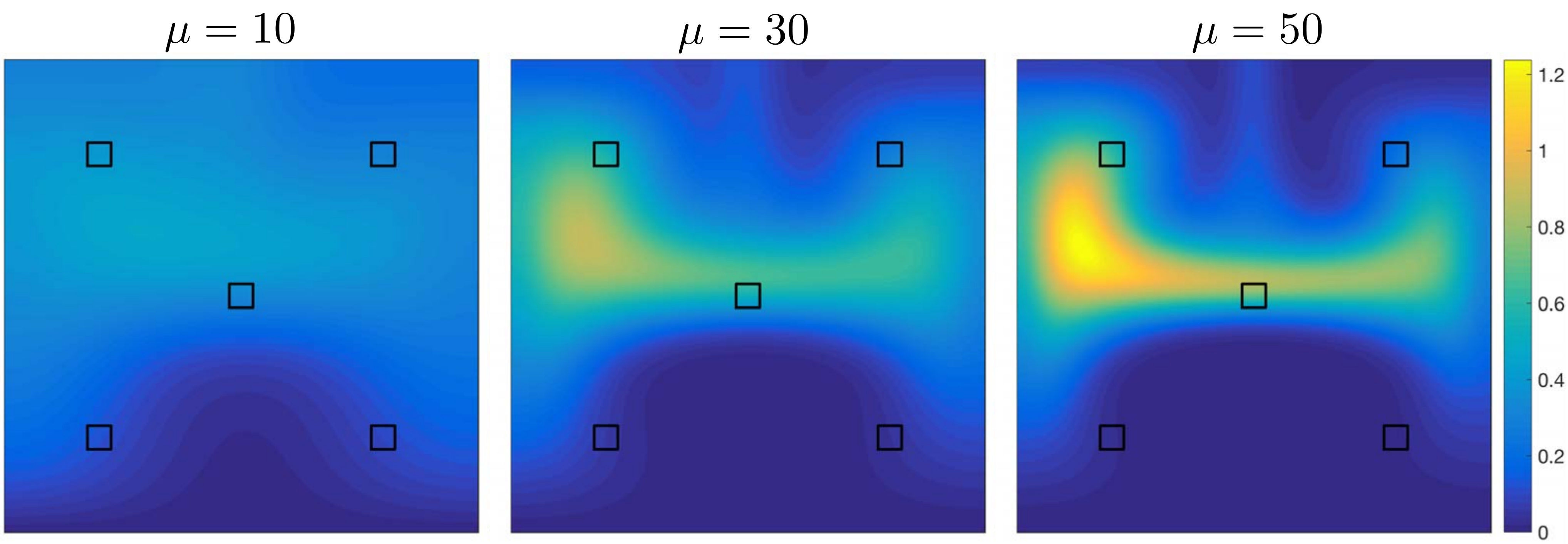
State variable $y(\mu)$



$k = 20$

Model Problem

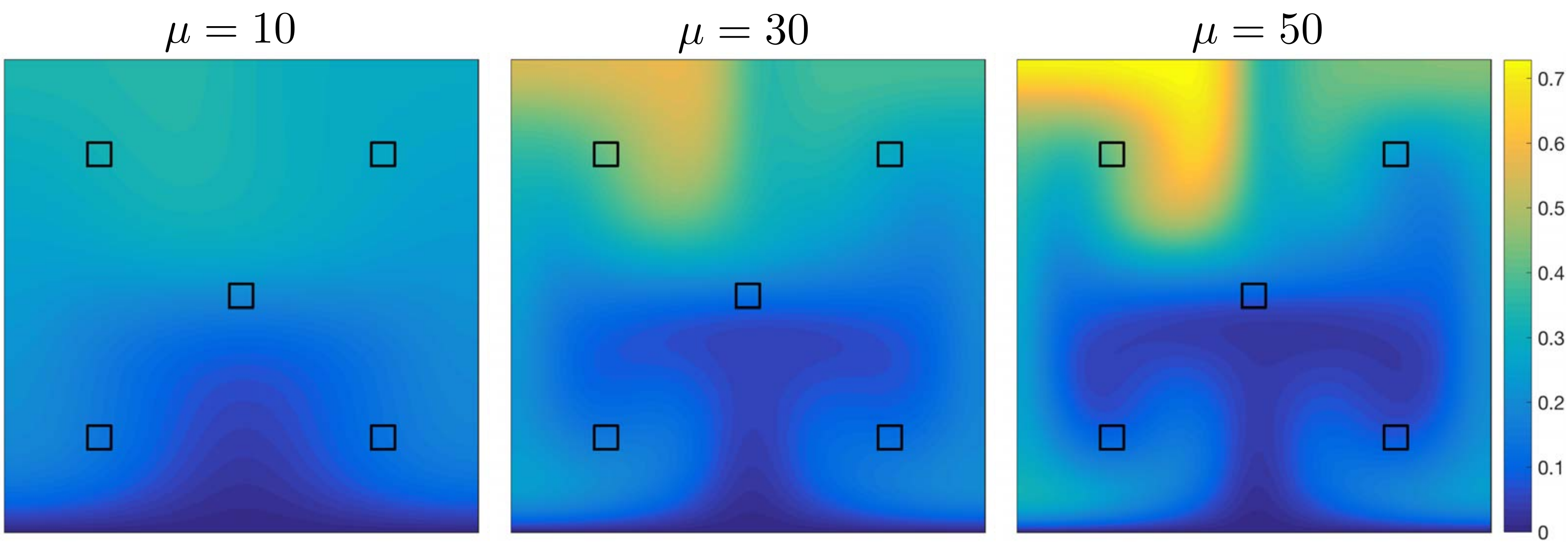
State variable $y(\mu)$



$k = 40$

Model Problem

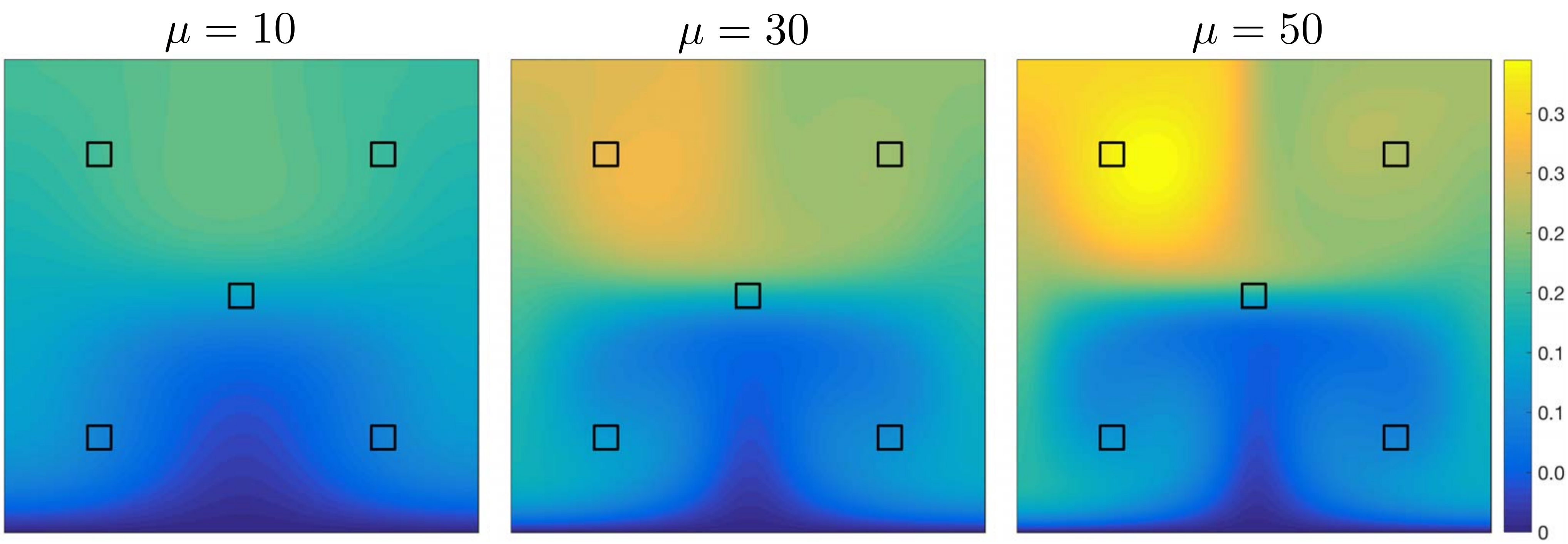
State variable $y(\mu)$



$k = 80$

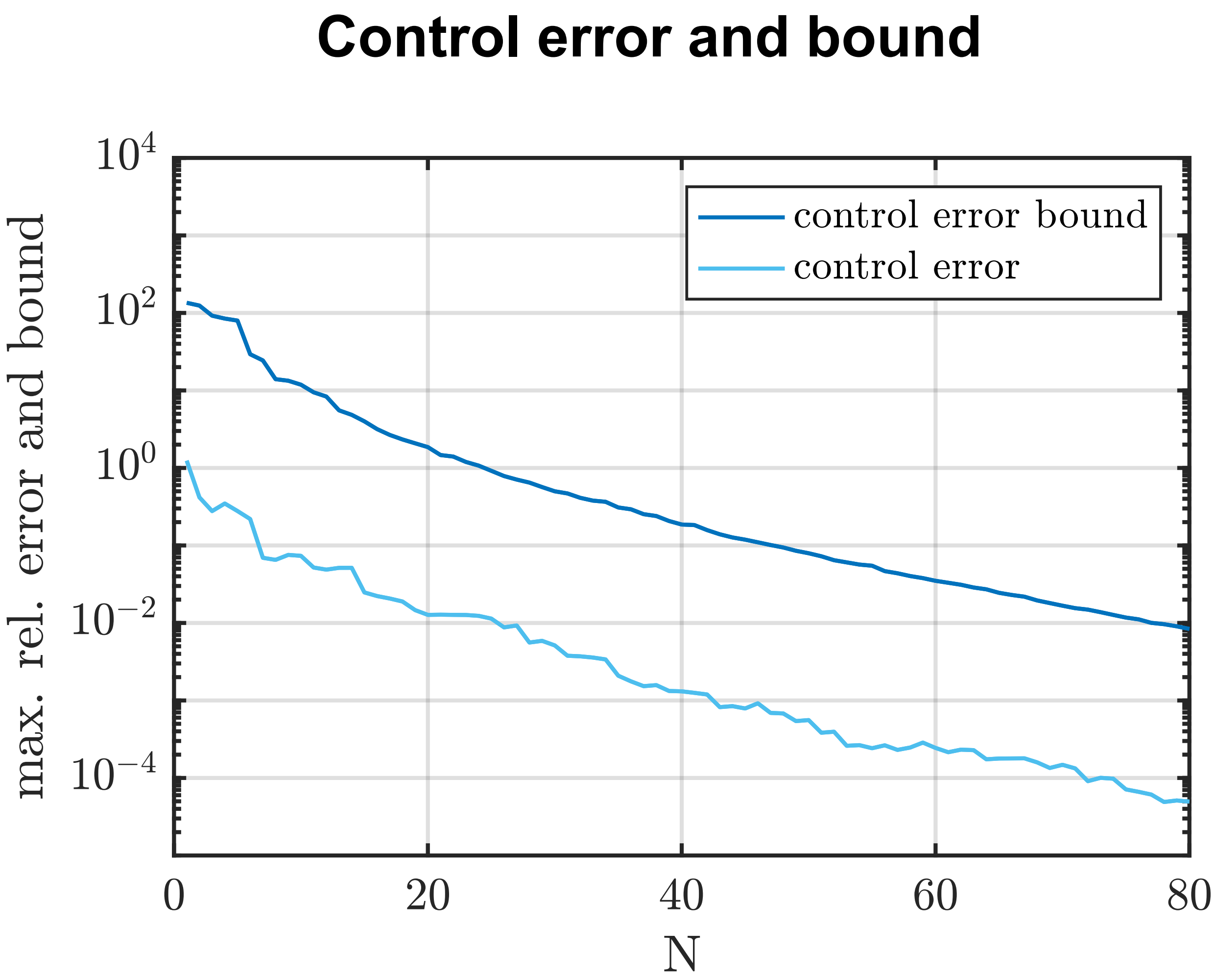
Model Problem

State variable $y(\mu)$



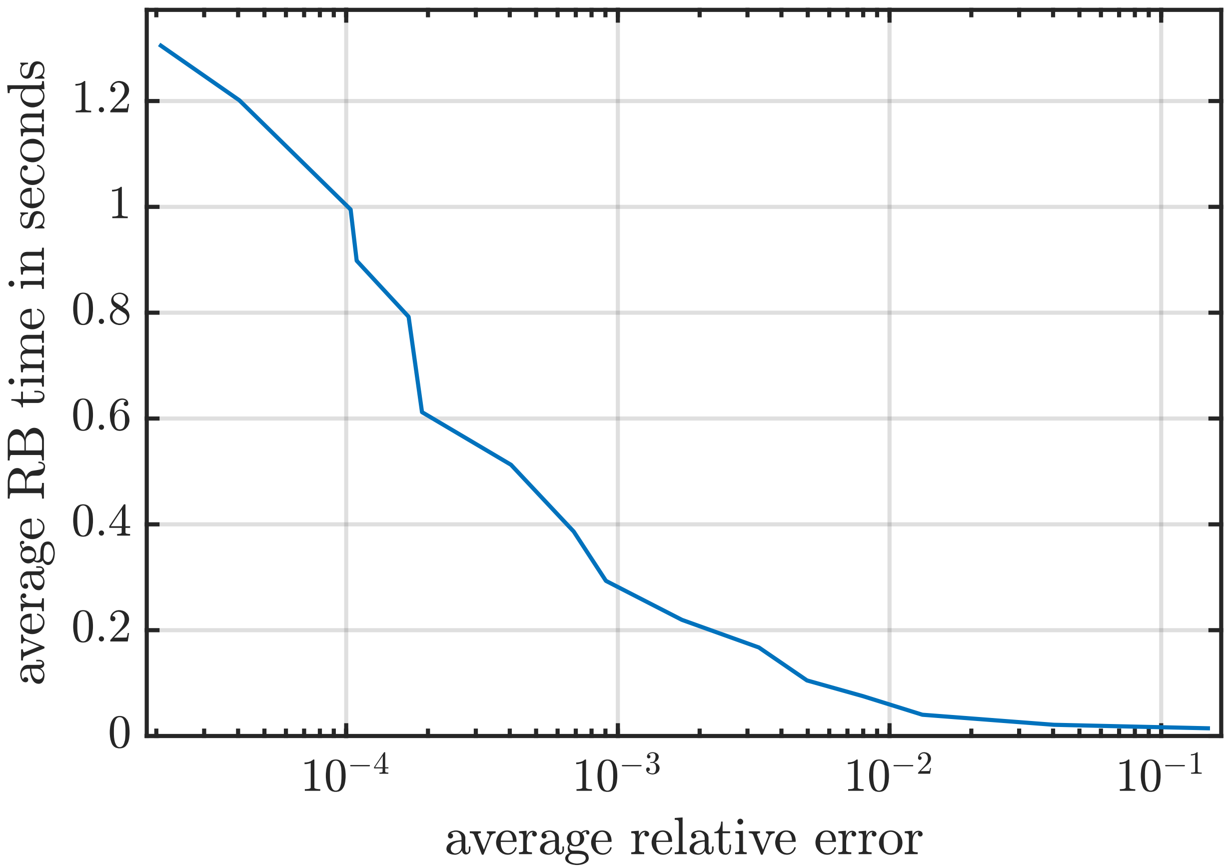
$k = 160$

Model Problem

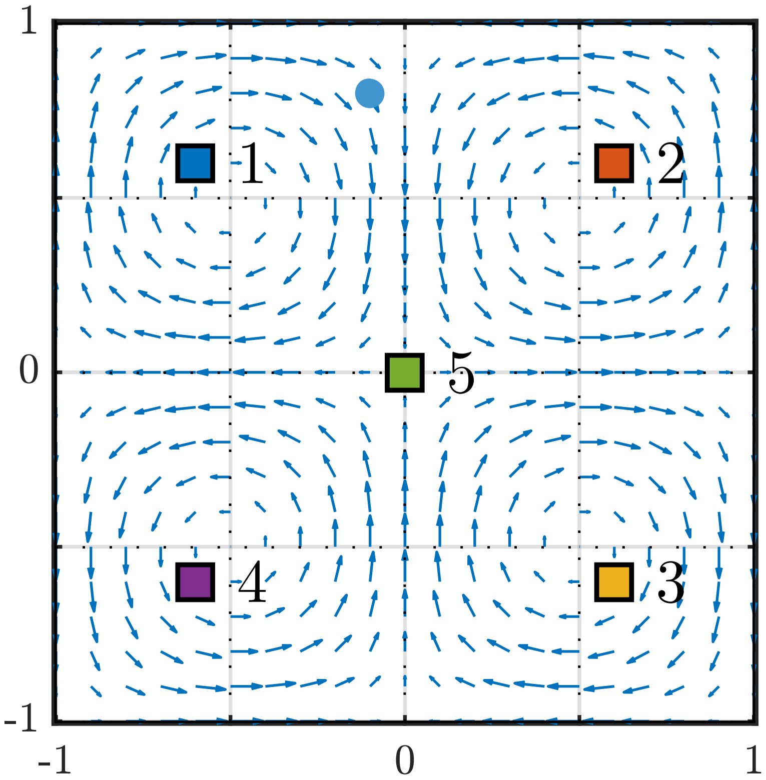


Model Problem

Computation Time



Model Problem



Contaminant transport

- “Gaussian” initial condition, $\bar{u}_0$
- Known Taylor-Green vortex velocity field
- Parameter $\mu = \mathrm{Pe} \in [10, 50], \bar{\mu} = 30$
- FE dimension $(\mathcal{N} = 13000, K = 200)$

Assumptions:

- Data generated with true initial condition
- Uncertainty due to noise,

  unknown parameter, **and model error**

Weak-constraint 4DVAR

$$\min_{u \in U} \quad \frac{1}{2}\sum_{k=1}^{K} \Delta t ||u^k||_{\Sigma}^2 + \frac{\lambda}{2}\sum_{k=1}^{K} \Delta t ||Cy^k - y_d^k||_D^2$$

$$\text{s.t.} \quad m(y^{k+1}, \nu) = m(y^k, \nu) - \Delta t\ a(y^k, \nu; \mu) + \Delta t\ f(\nu) + \Delta t\ m(u^k, \nu), \qquad \forall\, \nu \in Y,\ k = 1, \dots, K$$

$$y^0 = u^0$$

- Account for inexact model by adding a model error term, where

u^k	the model error in each time step
Σ	covariance of the model error

- Allows to consider longer analysis windows

A Posteriori Error Estimation

$$\left(\Delta t \sum_{k=1}^{K} \| u^{*,k} - u_N^{*,k} \|_{\mathcal{U}}^2 \right)^{1/2} \leq \tilde{\Delta}_N^u(\mu) := c_1(\mu) + \sqrt{c_1(\mu)^2 + c_2(\mu)}$$

$$\forall\, \mu \in \mathcal{D}$$

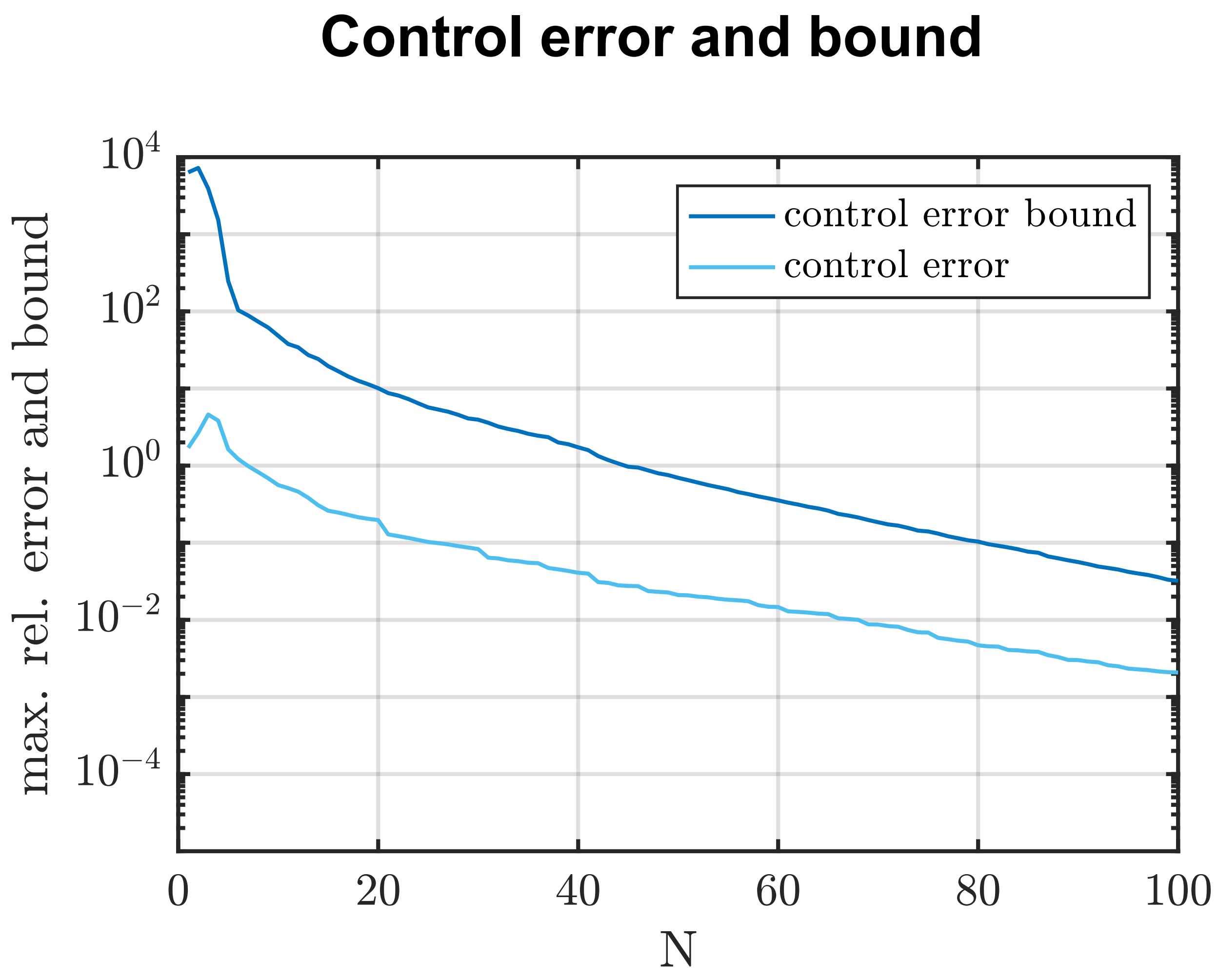
where

$$c_1(\mu) = \frac{1}{2} \left(\tilde{R}_u + \frac{\sqrt{2}\gamma_b}{\alpha_a^{\mathrm{LB}}} \tilde{R}_p \right)$$

$$c_2(\mu) = \frac{2\sqrt{2}}{\alpha_a^{\mathrm{LB}}} \tilde{R}_y \tilde{R}_p + \frac{\lambda \gamma_c^2}{2 \left(\alpha_a^{LB} \right)^2} \tilde{R}_y^2$$

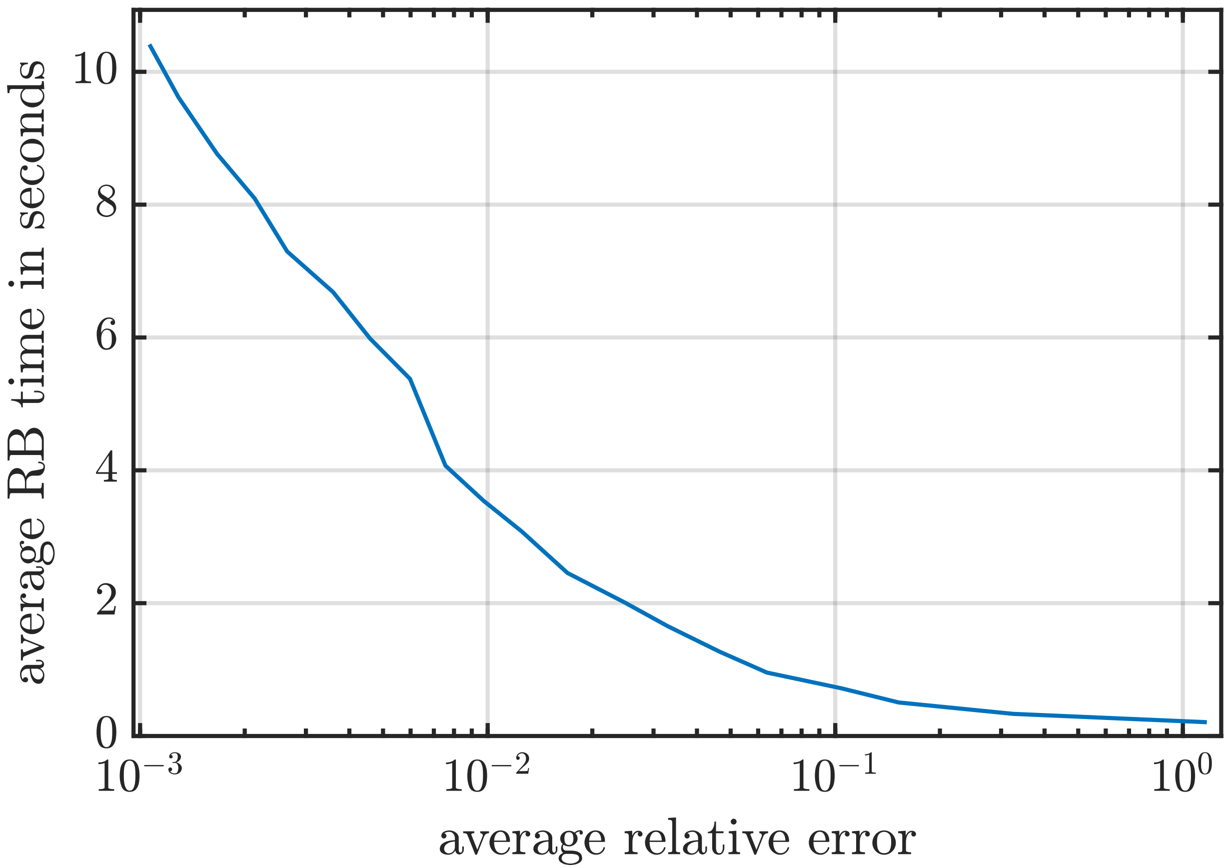
[Kärcher, Boyaval, Grepl, V., 2018]

Model Problem



Model Problem

Computation Time



4DVAR Summary

Key points

- Approximated solutions of the parametrized 4D-VAR problem using reduced basis methods
- Developed *a posteriori* error bounds for the error in the control (initial condition or model error) as well as state and adjoint
- Applied proposed methods to a simple parametrized convection-diffusion problem
- Estimated unknown parameter, initial condition, and model error

Issues and Perspectives

- Convergence and error estimates for the parameter estimation problem
- Introduce uncertainty in prior
- **Sensor placement**

Data Assimilation + Sensor Placement

with

N. Aretz-Nellesen and M. Grepl

Background

(Variational) Data Assimilation

3D-/4D-VAR	[Lorenc '81], [Le Dimet '81], [Courtier '85], …
	[Le Dimet & Talagrand '86], … [Navon et al] …
+ Kalman Filter, Bayesian Methods	[Law & Stuart '15], [Reich '15], …

MOR + Data Assimilation (+Sensor Placement)

Gappy-POD	[Everson & Sirovich '95], [Willcox '06] …
GEIM	[Maday & Mula '13] …
PGD (+ EIM)	[Nadal, Chinesta, Diez, Fuenmayor & Denia '15] …
PBDW	[**Maday, Patera, Penn & Yano '14**, '15], [Taddei '17],
	[**Maday & Taddei '17(p)**], [Taddei & Patera '18],
	[Hammond, Chaqir, Bourquin & Maday '18(p)]
OMP	[**Binev, Cohen, Mula & Nichols '18**]

MOR + Optimal Control

RB + OC	[Negri, Rozza, Manzoni, Quarteroni '13],
	[Tröltzsch & Volkwein '09], [Kärcher, Tokoutsi, Grepl & V. '18]

4DVAR

4DVAR (μ)

$$\min_{\mu\in\mathcal{D}} \min_{u\in\mathcal{U}} \quad \frac{1}{2}\|u-u_b\|_{\mathcal{U}}^2 \quad + \quad \frac{\lambda}{2}\sum_{k=1}^{K}\Delta t\|Cy^k - y_d^k\|_D^2$$

$$\text{s.t.} \quad m(y^k,\nu) = m(y^{k-1},\nu) - \Delta t\, a(y^k,\nu;\mu) + \Delta t\ f(\nu),$$

$$\forall\, \nu \in Y,\ k=1,\dots,K$$

$$y^0 = u$$

Solve for $\mu^*$and the estimate $(u^*(\mu^*), y^*(\mu^*))$.

3D-VAR

Modified Formulation

$$\min_{u \in \mathcal{U}} \frac{1}{2}\|u\|_{\mathcal{U}}^2 + \frac{\lambda}{2}\|d\|_{\mathcal{Y}}^2$$

$$\text{s.t.} \quad a(y,v) = f(v) + b(u,v) \quad \forall v \in \mathcal{Y} \qquad (\mathcal{M})$$

$$(y + d, \tau)_{\mathcal{Y}} = (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} \quad \forall \tau \in \mathcal{T} \subset \mathcal{Y}$$

where

u	model bias
d	misfit between state and “data"
y	state
y_{d}	"data"
λ	regularisation parameter
$\mathcal{M}$	is the best- knowledge model of the physics.

3D-VAR

Modified Formulation

$$\min_{u \in \mathcal{U}} \frac{1}{2}\|u\|_{\mathcal{U}}^2 + \frac{\lambda}{2}\|d\|_{\mathcal{Y}}^2$$

$$\text{s.t.} \quad a(y,v) = f(v) + b(u,v) \quad \forall v \in \mathcal{Y} \qquad (\mathcal{M})$$

$$(y + d, \tau)_{\mathcal{Y}} = (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} \quad \forall \tau \in \mathcal{T} \subset \mathcal{Y}$$

Variational Data Assimilation

- Prevalent in meteorology and oceanography

  [Law & Stuart 2015], [Reich 2015],…

- Given a best knowledge model and data

  find (allowed) perturbations u to the model

  such that u and the misfit d are as small as possible.

Introduction to Reduced Basis Methods: Theory and Applications |
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Aachen Institute for Advanced Study in Computational Engineering Science
RWTH AACHEN UNIVERSITY

3D-VAR

Modified Formulation

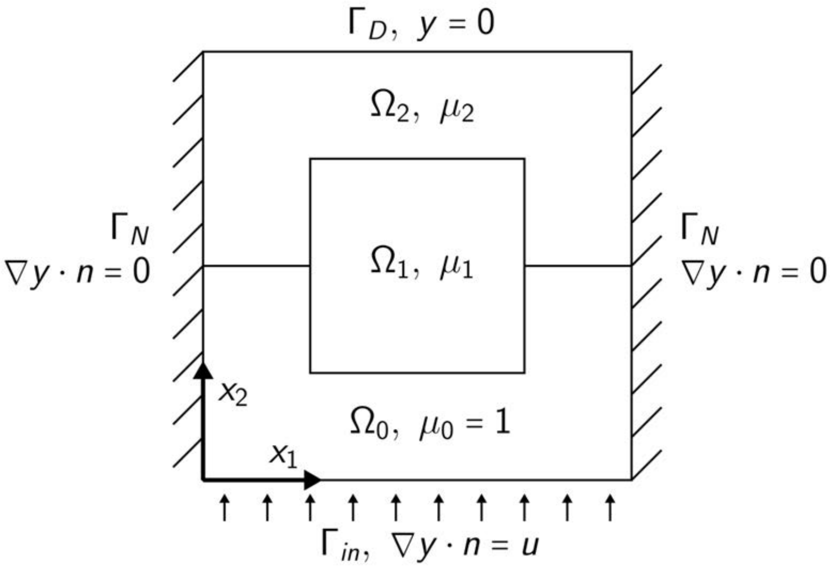
$$\left(\min_{\mu\in\mathcal{D}}\right) \min_{u\in\mathcal{U}} \frac{1}{2}\|u(\mu)\|_{\mathcal{U}}^2 + \frac{\lambda}{2}\|d(\mu)\|_{\mathcal{Y}}^2$$

$$\text{s.t.} \quad a(y(\mu), v; \mu) = f(v;\mu) + b(u(\mu), v) \qquad \forall v \in \mathcal{Y}$$

$$(y(\mu) + d(\mu), \tau)_{\mathcal{Y}} = (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} \qquad \forall \tau \in \mathcal{T} \subset \mathcal{Y}$$

Issues

- Bias in boundary conditions
- Error in model form
- Unknown or uncertain parameters
- Noisy data



3D-VAR

Modified Formulation

$$\left(\min_{\mu\in\mathcal{D}}\right) \min_{u\in\mathcal{U}} \frac{1}{2}\|u(\mu)\|_{\mathcal{U}}^2 + \frac{\lambda}{2}\|d(\mu)\|_{\mathcal{Y}}^2$$

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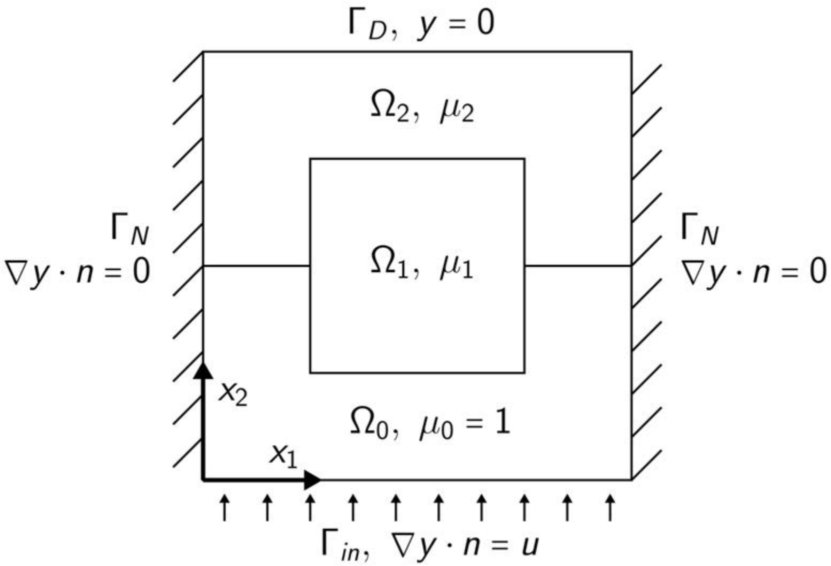

3D-VAR

Modified Formulation

$$\left(\min_{\mu\in\mathcal{D}}\right) \min_{u\in\mathcal{U}} \frac{1}{2}\|u(\mu)\|_{\mathcal{U}}^2 + \frac{\lambda}{2}\|d(\mu)\|_{\mathcal{Y}}^2$$

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$$(y(\mu) + d(\mu), \tau)_{\mathcal{Y}} = (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} \qquad \forall \tau \in \mathcal{T} \subset \mathcal{Y}$$

Relation to Optimal Control

[Nellesen '18(MS)]

- Distributed optimal control (+ minimization problem)
- $b(u, v)$ represents permitted corrections to the model
- Optimality leads to saddle point structure
- Use RB approximation, error bounds in [Kärcher, Tokoutsi, Grepl & V. '17]
- Difference: Measurement space $\mathcal{T} \subset \mathcal{Y}$

3D-VAR + RB

Modified Formulation

$$\left(\min_{\mu\in\mathcal{D}}\right) \min_{u_N \in \mathcal{U}_N} \frac{1}{2}\|u_N(\mu)\|^2_{\mathcal{U}} + \frac{\lambda}{2}\|d_N(\mu)\|^2_{\mathcal{Y}}$$

$$\text{s.t.} \quad a(y_N(\mu), v; \mu) = f(v;\mu) + b(u_N(\mu), v) \quad \forall v \in \mathcal{Y}_N$$

$$(y_N(\mu) + d_N(\mu), \tau)_{\mathcal{Y}} = (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} \quad \forall \tau \in \mathcal{T}$$

Reduced Basis Approximation

[Nellesen '18(MS)]

- Introduce reduced spaces for control, state, and adjoints
- Galerkin projection onto reduced basis spaces
- A posteriori error bounds for control, state, adjoint, and misfit
- Offline / online decomposition
- Greedy algorithm to construct approximation spaces

3D-VAR + RB Error Estimation

Residuals

To obtain an *a posteriori* error bound for each error term

$$e_u := u^* - u_N^*, \qquad e_y := y^* - y_N^*, \qquad e_d := d^* - d_N^*, \qquad e_p := p^* - p_N^*,$$

(control) (state) (misfit) (adjoint)

we define the residuals

$$\begin{aligned}
r_u : \mathcal{U} \to \mathbb{R} \qquad r_u(\phi) \quad &:= \quad b + \mu(\phi, p_N^*) - (u_N^*, \phi)_{\mathcal{U}} \\
r_p : \mathcal{Y} \to \mathbb{R} \qquad r_p(\psi) \quad &:= \quad \lambda(\psi, d_N^*)_{\mathcal{Y}} - a_\mu(\psi, p_N^*) \\
r_y : \mathcal{Y} \to \mathbb{R} \qquad r_y(\psi) \quad &:= \quad f_\mu(\psi) + b_\mu(u_N^*, \psi) - a_\mu(y_N^*, \psi)
\end{aligned}$$

whose norms can be computed in an *offline-online* procedure.

3D-VAR + RB Error Estimation

A Posteriori Error Bounds

Define further

$$g_u := \|r_u\|_{\mathcal{U}'} + \frac{1}{\alpha_\mu}\|b_\mu\|\|r_p\|_{\mathcal{Y}'} \qquad g_d := \frac{1}{\alpha_\mu}\|r_y\|_{\mathcal{Y}'}$$

$$h_u := \frac{2}{\alpha_u}\|r_p\|_{\mathcal{Y}'}\|r_y\|_{\mathcal{Y}'} + \frac{\lambda}{4\alpha_\mu^2}\|r_y\|_{\mathcal{Y}'}^2 \qquad h_d := \frac{2}{\lambda\alpha_\mu}\|r_p\|_{\mathcal{Y}'}\|r_y\|_{\mathcal{Y}'} + \frac{1}{4\lambda}g_u^2$$

Then

$$\|e_u\|_{\mathcal{Y}} \leqslant \tfrac{1}{2}g_u + \sqrt{\tfrac{1}{4}g_u^2 + h_u} \qquad \|e_y\|_{\mathcal{U}} \leqslant \frac{1}{\alpha_\mu}\|r_y\|_{\mathcal{Y}'} + \frac{\|b_\mu\|}{\alpha_\mu}\|e_u\|_{\mathcal{U}}$$

$$\|e_d\|_{\mathcal{Y}} \leqslant \tfrac{1}{2}g_d + \sqrt{\tfrac{1}{4}g_d^2 + h_d} \qquad \|e_p\|_{\mathcal{U}} \leqslant \frac{1}{\alpha_\mu}\|r_p\|_{\mathcal{Y}'} + \frac{\lambda}{\alpha_\mu}\|e_d\|_{\mathcal{U}}$$

Similar *a posteriori* error bounds in [Kärcher, Tokoutsi, Grepl & V. '18]

3D-VAR

Modified Formulation

$$\left(\min_{\mu \in \mathcal{D}}\right) \min_{u \in \mathcal{U}} \frac{1}{2}\|u(\mu)\|_{\mathcal{U}}^2 + \frac{\lambda}{2}\|d(\mu)\|_{\mathcal{Y}}^2$$

$$\text{s.t.} \quad a(y(\mu), v; \mu) = f(v; \mu) + b(u(\mu), v) \quad \forall v \in \mathcal{Y}$$

$$(y(\mu) + d(\mu), \tau)_{\mathcal{Y}} = (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} \quad \forall \tau \in \mathcal{T} \subset \mathcal{Y}$$

How do we optimally select the measurements?

3D-VAR

Modified Formulation

$$\left(\min_{\mu\in\mathcal{D}}\right) \min_{u\in\mathcal{U}} \frac{1}{2}\|u(\mu)\|_{\mathcal{U}}^2 + \frac{\lambda}{2}\|d(\mu)\|_{\mathcal{Y}}^2$$

$$\begin{aligned} \text{s.t.} \quad & a(y(\mu), v; \mu) = f(v; \mu) + b(u(\mu), v) && \forall v \in \mathcal{Y} \\ & (y(\mu) + d(\mu), \tau)_{\mathcal{Y}} = (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} && \forall \tau \in \mathcal{T} \subset \mathcal{Y} \end{aligned}$$

How do we optimally select the measurement space $\mathcal{T}$

where $\mathcal{T}$ is the space spanned by the Riesz representation

of the measurement functionals?

$\longrightarrow$ Stability analysis

[Maday, Patera, Penn & Yano '14]

3D-VAR(μ): Stability Analysis

One can show that

$$\|(u_\mu^*, y_\mu^*)(\lambda)\|_{\mathcal{U}\times\mathcal{Y}} \leqslant C_1^\mu(\lambda)\|y_\mathrm{d}\|_{\mathcal{Y}} + C_2^\mu(\lambda)\|f_{\mathrm{bk},\mu}\|_{\mathcal{Y}'}$$

$$\|p_\mu^*(\lambda)\|_{\mathcal{Y}} \leqslant C_3^\mu(\lambda)\|y_\mathrm{d}\|_{\mathcal{Y}} + C_4^\mu(\lambda)\|f_{\mathrm{bk},\mu}\|_{\mathcal{Y}'}$$

with positive stability constants.

The stability constants are “better-behaved” for [Nellesen et al. '18(p)]

$$\underline{\eta}(\mu) := \inf_{(u,y)\in\mathcal{H}^0(\mu)} \frac{\|y\|_{\mathcal{Y}}}{\|u\|_{\mathcal{U}}} \overset{!}{>} 0 \qquad \beta_{\mathcal{T}}(\mu) := \inf_{y\in\mathcal{Y}_\mu} \sup_{\tau\in\mathcal{T}} \frac{(y,\tau)_{\mathcal{Y}}}{\|y\|_{\mathcal{Y}}\|\tau\|_{\mathcal{Y}}} \overset{!}{>} 0$$

as large as possible. Here,

$$\begin{aligned}
\mathcal{H}^0(\mu) &:= \{\, (u,y) \in \mathcal{U}\times\mathcal{Y} : a_\mu(y,\psi) = b_\mu(u,\psi) \quad \forall\psi\in\mathcal{Y} \,\},\\
\mathcal{Y}_\mu &:= \{\, y\in\mathcal{Y} : \exists\, u\in\mathcal{U} \text{ s.t. } a_\mu(y,\psi) = b_\mu(u,\psi) \quad \forall\psi\in\mathcal{Y} \,\}.
\end{aligned}$$

3D-VAR(μ): Stability Analysis

One can show that

$$\|(u_\mu^*, y_\mu^*)(\lambda)\|_{\mathcal{U}\times\mathcal{Y}} \leqslant C_1^\mu(\lambda)\|y_{\mathrm{d}}\|_{\mathcal{Y}} + C_2^\mu(\lambda)\|f_{\mathrm{bk},\mu}\|_{\mathcal{Y}'}$$

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3DVAR + RB

Modified Formulation

$$\left(\min_{\mu\in\mathcal{D}}\right) \min_{u\in\mathcal{U}} \tfrac{1}{2}\|u(\mu)\|_{\mathcal{U}}^2 + \tfrac{\lambda}{2}\|d(\mu)\|_{\mathcal{Y}}^2$$

$$\begin{aligned} \text{s.t.} \quad & a(y(\mu), v; \mu) = f(v;\mu) + b(u(\mu), v) && \forall v \in \mathcal{Y} \\ & (y(\mu) + d(\mu), \tau)_{\mathcal{Y}} = (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} && \forall \tau \in \mathcal{T} \end{aligned}$$

3DVAR + RB

Modified Formulation

$$\left(\min_{\mu\in\mathcal{D}}\right) \min_{u\in\mathcal{U}} \tfrac{1}{2}\|u_N(\mu)\|^2_{\mathcal{U}} + \tfrac{\lambda}{2}\|d_N(\mu)\|^2_{\mathcal{Y}}$$

$$\begin{aligned} \text{s.t.} \qquad & a(y_N(\mu), v; \mu) = f(v;\mu) + b(u_N(\mu), v) && \forall v \in \mathcal{Y}_N \\ & (y_N(\mu) + d_N(\mu), \tau)_{\mathcal{Y}} = (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} && \forall \tau \in \mathcal{T} \end{aligned}$$

Assume that

[Nellesen, Grepl & V. '18(p)]

$$\|y - y_N\|_{\mathcal{Y}} \leqslant \varepsilon_\mu \|y\|_{\mathcal{Y}} \quad \text{where } 0 \leqslant \varepsilon_\mu \ll 1$$

Then

$$\beta_{\mathcal{T}}(\mu) \geqslant (1-\varepsilon_\mu)\beta_{\mathcal{T},N}(\mu) - \varepsilon_\mu$$

Construction of RB Spaces

Procedure

Recall optimality conditions [Nellesen, Grepl & V. '18]

$$
\begin{aligned}
(u^*_\mu, \phi)_{\mathcal{U}} - b_\mu(\phi, p^*_\mu) &= 0 && \forall \quad \phi \in \mathcal{U} && \text{control} \\
a_\mu(\psi, p^*_\mu) - \lambda(\psi, d^*_\mu)_{\mathcal{Y}} &= 0 && \forall \quad \psi \in \mathcal{Y} && \text{adjoint} \\
a_\mu(y^*_\mu, \psi) - b_\mu(u^*_\mu, \psi) &= f_{\mathrm{bk},\mu}(\psi) && \forall \quad \psi \in \mathcal{Y} && \text{state} \\
(y^*_\mu + d^*_\mu, \tau)_{\mathcal{Y}} &= (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} && \forall \quad \tau \in \mathcal{T}. && \text{misfit}
\end{aligned}
$$

Construction of RB Spaces

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Recall optimality conditions [Nellesen, Grepl & V. '18]

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\begin{array}{rclll}
(u^*_\mu, \phi)_{\mathcal{U}} - b_\mu(\phi, p^*_\mu) & = & 0 & \forall \quad \phi \in \mathcal{U} & \text{control} \\
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(y^*_\mu + d^*_\mu, \tau)_{\mathcal{Y}} & = & (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} & \forall \quad \tau \in \mathcal{T}. & \text{misfit}
\end{array}
$$

$$
\mathcal{U}_N \longrightarrow \mathcal{Y}_{y,N} \longrightarrow \mathcal{T} \longrightarrow \mathcal{Y}_{p,N} \longrightarrow \mathcal{Y}_N = \mathcal{Y}_{y,N} + \mathcal{Y}_{p,N}
$$

Given a low dimensional approximation to the space of model corrections (i.e., control)

Construction of RB Spaces

Procedure

Recall optimality conditions [Nellesen, Grepl & V. '18]

$$
\begin{array}{rcllr}
(u_\mu^*, \phi)_{\mathcal{U}} - b_\mu(\phi, p_\mu^*) & = & 0 & \forall \ \phi \in \mathcal{U} & \text{control} \\
a_\mu(\psi, p_\mu^*) - \lambda(\psi, d_\mu^*)_{\mathcal{Y}} & = & 0 & \forall \ \psi \in \mathcal{Y} & \text{adjoint} \\
\boxed{a_\mu(y_\mu^*, \psi) - b_\mu(u_\mu^*, \psi) = f_{\mathrm{bk},\mu}(\psi) \quad \forall \ \psi \in \mathcal{Y} \quad \text{state}} \\
(y_\mu^* + d_\mu^*, \tau)_{\mathcal{Y}} & = & (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} & \forall \ \tau \in \mathcal{T}. & \text{misfit}
\end{array}
$$

$$\mathcal{U}_N \longrightarrow \mathcal{Y}_{y,N} \longrightarrow \mathcal{T} \longrightarrow \mathcal{Y}_{p,N} \longrightarrow \mathcal{Y}_N = \mathcal{Y}_{y,N} + \mathcal{Y}_{p,N}$$

Construct an RB space for the state
Note that $\mathcal{T}$ is not yet required!

Construction of RB Spaces

Procedure

Recall optimality conditions [Nellesen, Grepl & V. '18]

$$
\begin{array}{rcllr}
(u_\mu^*, \phi)_{\mathcal{U}} - b_\mu(\phi, p_\mu^*) & = & 0 & \forall \ \phi \in \mathcal{U} & \text{control} \\
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\end{array}
$$

$$
\mathcal{U}_N \longrightarrow \mathcal{Y}_{y,N} \longrightarrow \mathcal{T} \longrightarrow \mathcal{Y}_{p,N} \longrightarrow \mathcal{Y}_N = \mathcal{Y}_{y,N} + \mathcal{Y}_{p,N}
$$

Select optimal measurements via
greedy algorithm in the parameter domain +
orthogonal matching pursuit [Binev et al. '18]

Construction of RB Spaces

Procedure

Recall optimality conditions [Nellesen, Grepl & V. '18]

$$
\begin{array}{rclll}
(u_\mu^*, \phi)_{\mathcal{U}} - b_\mu(\phi, p_\mu^*) & = & 0 & \forall \quad \phi \in \mathcal{U} & \text{control} \\
\boxed{a_\mu(\psi, p_\mu^*) - \lambda(\psi, d_\mu^*)_{\mathcal{Y}} = 0 \quad \forall \quad \psi \in \mathcal{Y} \quad \text{adjoint}} & & & & \\
a_\mu(y_\mu^*, \psi) - b_\mu(u_\mu^*, \psi) & = & f_{\mathrm{bk},\mu}(\psi) & \forall \quad \psi \in \mathcal{Y} & \text{state} \\
(y_\mu^* + d_\mu^*, \tau)_{\mathcal{Y}} & = & (y_{\mathrm{d}}, \tau)_{\mathcal{Y}} & \forall \quad \tau \in \mathcal{T}. & \text{misfit}
\end{array}
$$

$$
\mathcal{U}_N \longrightarrow \mathcal{Y}_{y,N} \longrightarrow \mathcal{T} \longrightarrow \mathcal{Y}_{p,N} \longrightarrow \mathcal{Y}_N = \mathcal{Y}_{y,N} + \mathcal{Y}_{p,N}
$$

Construct an RB space for the adjoint

Numerical Experiment

Thermal Block

- State space

$\mathcal{Y}$ FE-discretization of

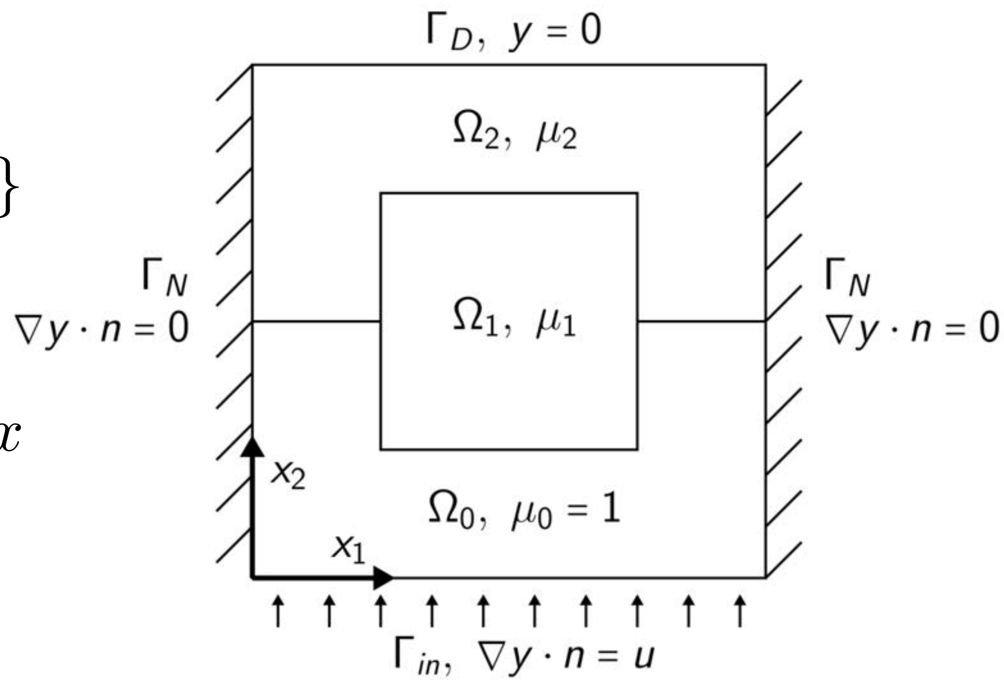
$$\mathcal{Y}_{\mathrm{e}} := \{y \in H^1(\Omega) : y|_{\Gamma_{\mathrm{D}}} = 0\}$$

- Bilinear form

$$a_\mu(y, w) := \sum_{i=0}^{2} \mu_i \int_{\Omega_i} \nabla y \cdot \nabla w \, dx$$

- Parameter domain

$$\mathcal{C} := [0.1, 10]^2$$



Numerical Experiment

Thermal Block

- Source term

$$b(u,\cdot) \in \mathcal{Y}',\; b(u,w) := \int_{\Gamma_{\text{in}}} uw \; dS,$$

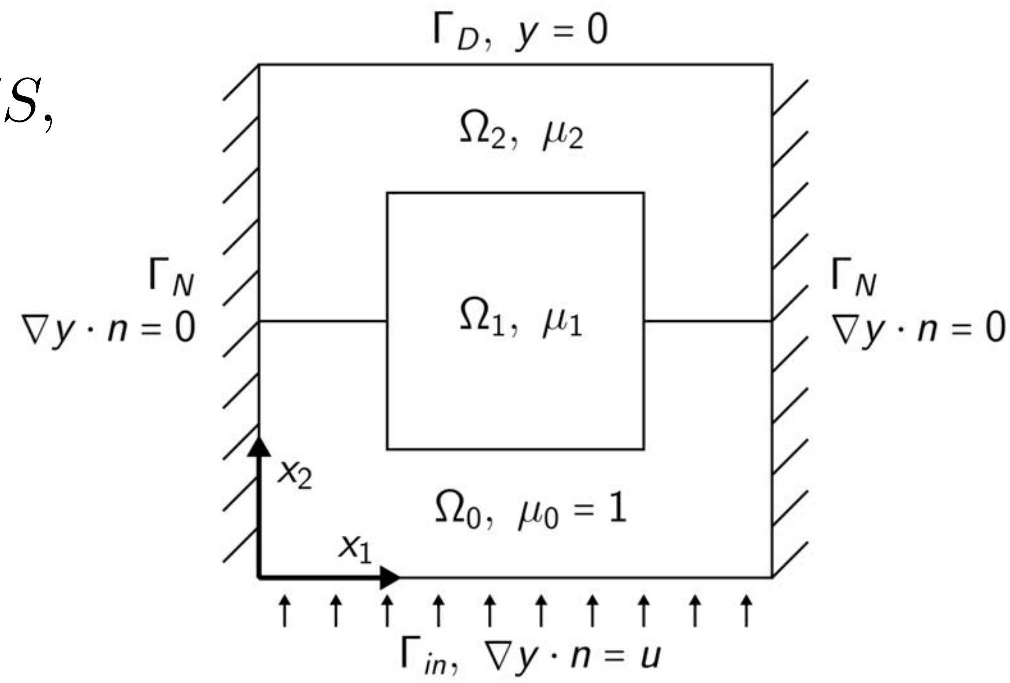
where $u \in L^2(\Gamma_{\text{in}})$

- BK-model source term

$$f_{\text{bk},\mu} = b(u_{\text{bk}},\cdot),\; u_{\text{bk}} \equiv 1$$

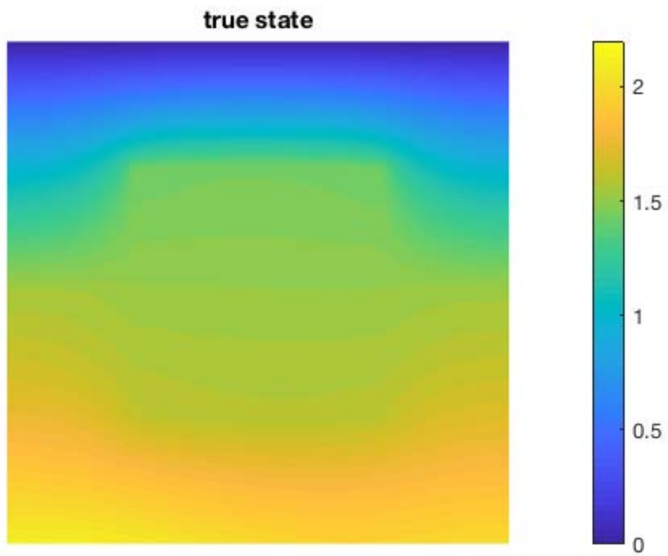
- Model correction

$\mathcal{U} = \mathbb{P}_3$ (polynomial space)



Numerical Experiment

Parameter Estimation Problem Statement



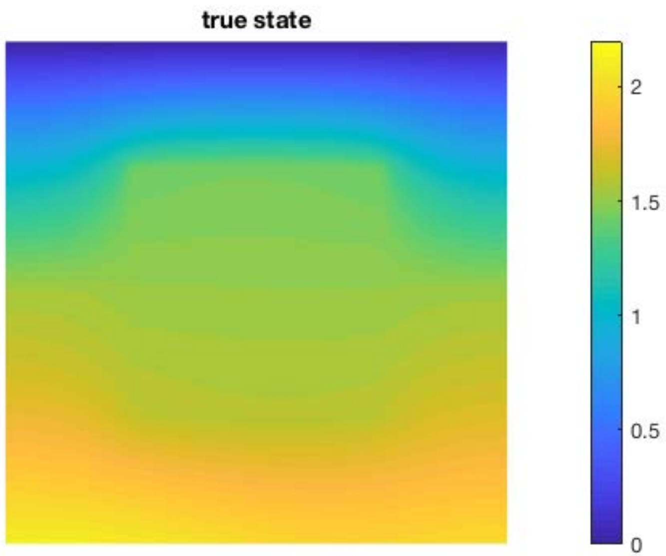
Approximate the unknown variables

- $\mu_{\text{true}} = (7, 0.3) \in \mathcal{C}$
- $u_{\text{true}}(x) \approx 1.5 + 0.3\sin(2\pi x), \;\; x \in \Gamma_{\text{in}}$
- $y_{\text{true}} = y_{\mu_{\text{true}}}(u_{\text{true}})$

with the 3D-VAR solution.

Numerical Experiment

Parameter Estimation Problem Statement



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- $y_{\text{true}} = y_{\mu_{\text{true}}}(u_{\text{true}})$

with the 3D-VAR solution.

Prior Knowledge:

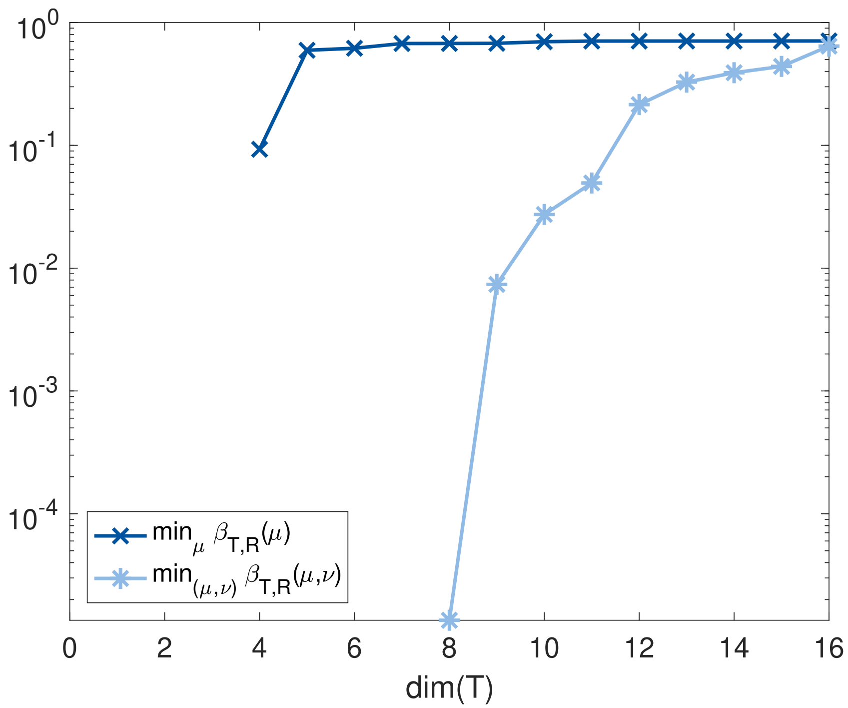
u_{true} can be approximated in $\mathcal{U} := \mathcal{P}_3$ sufficiently

Measurement Space:

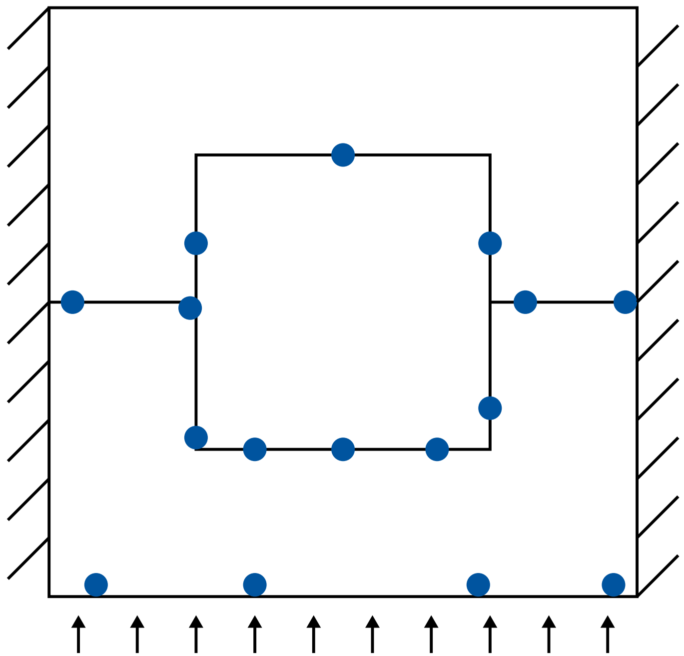
A small number of measurements may be chosen from a library of
gaussian functionals with std. dev. 0.01 and centers within $(0.02, 0.98)^2 \subset \Omega$

Numerical Results

Selection of the Measurement Space



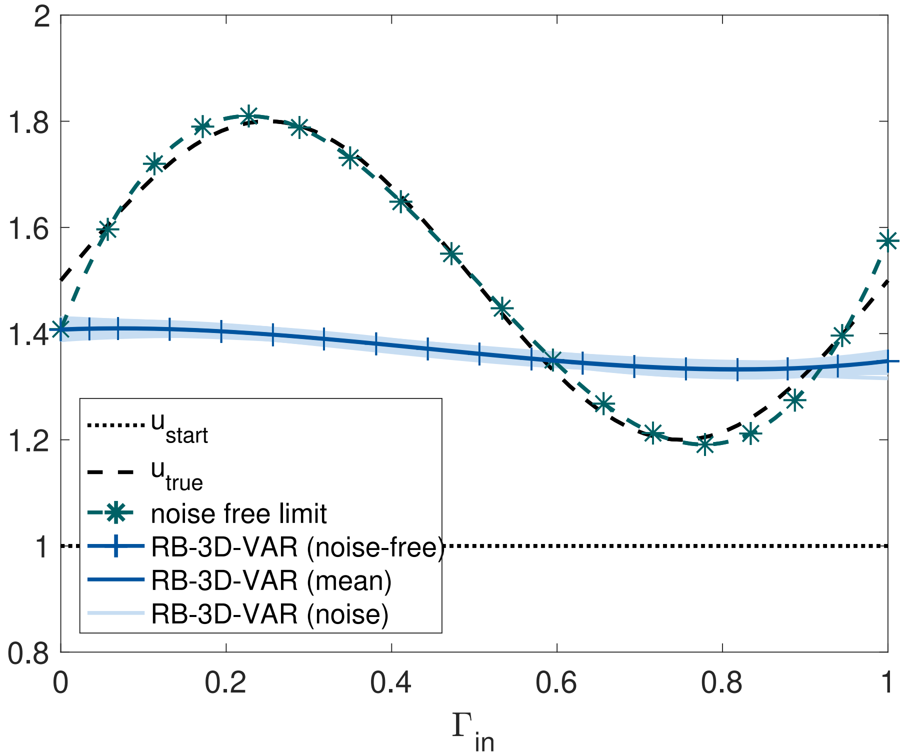
inf-sup constants during measurement selection



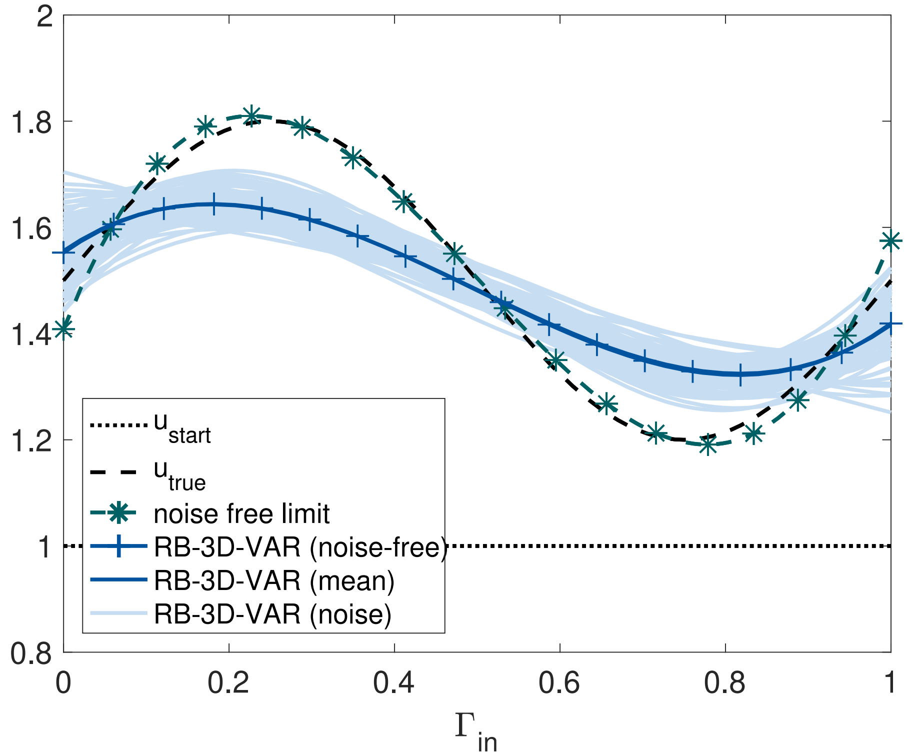
chosen measurement centers

Numerical Results

3D- VAR model correction



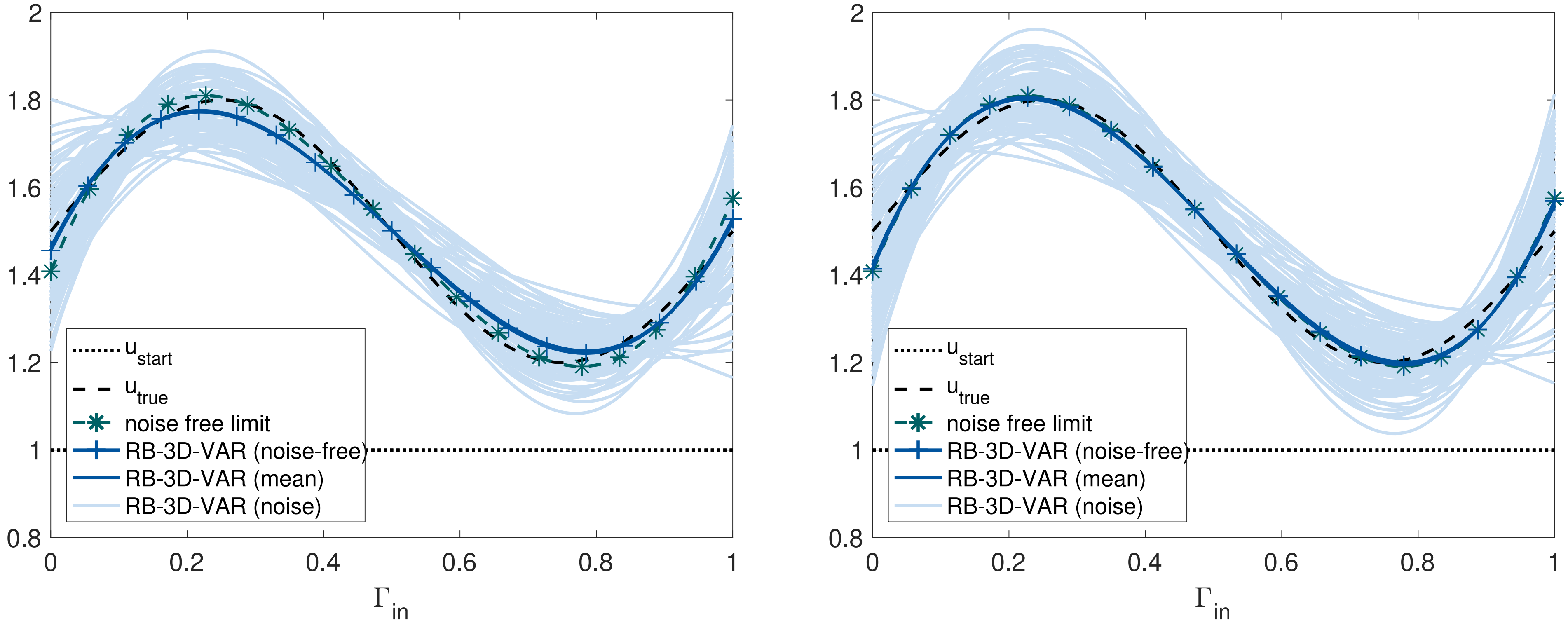
$\lambda = 1$



$\lambda = 10$

Numerical Results

3D- VAR model correction



λ = 100 λ = 1000

Numerical Results

Reduced Basis Spaces

$$\mathcal{U}_N \longrightarrow \mathcal{Y}_{y,N} \longrightarrow \mathcal{T} \longrightarrow \mathcal{Y}_{p,N} \longrightarrow \mathcal{Y}_N = \mathcal{Y}_{y,N} + \mathcal{Y}_{p,N}$$

Space dimensions:

	$\mathcal{U}$	$\mathcal{Y}_y$	$\mathcal{Y}_y$	$\mathcal{Y}_R$	$\mathcal{T}$
dim	4	64	95	159	16

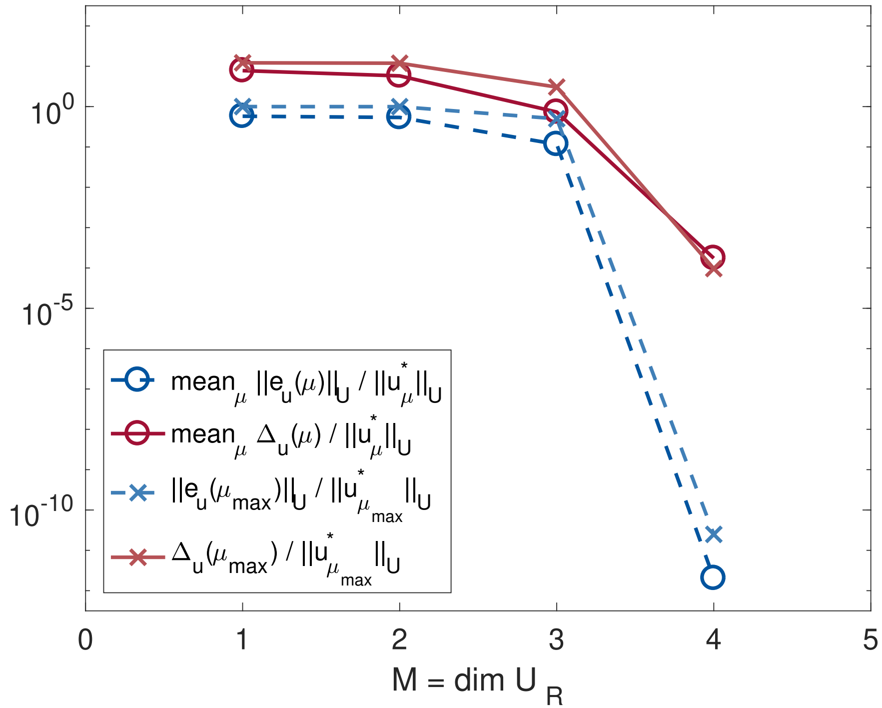
Computational time:

FE-3D-VAR	RB-3D-VAR			speedup
	offline	online	error bound	
7.08 s	463 s	4.2 ms	1.3 ms	1,276

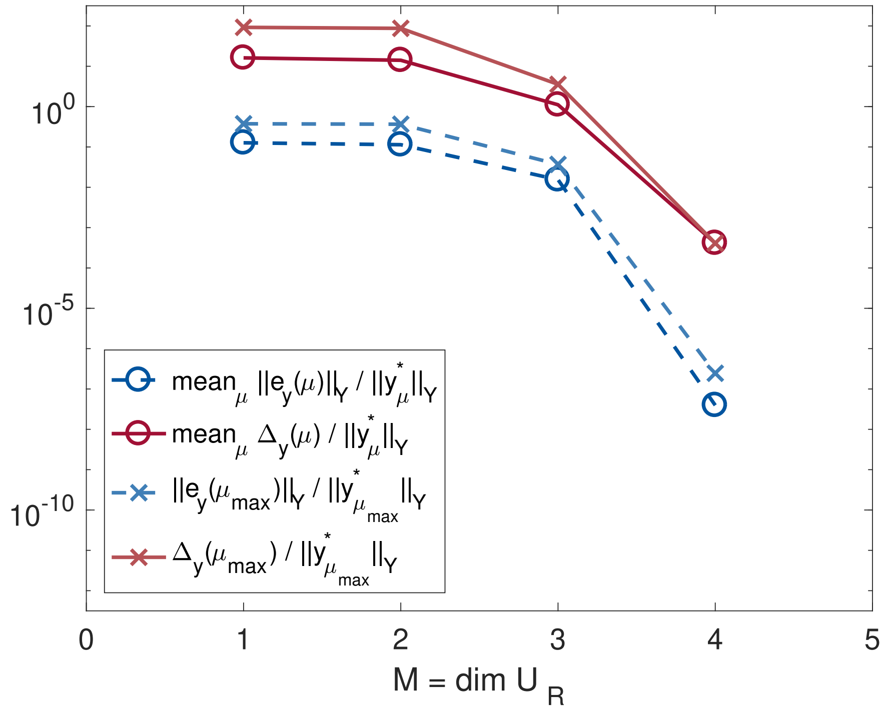
Parameter estimation: roughly 25-28 mins.

Numerical Results

A Posteriori Error Bounds



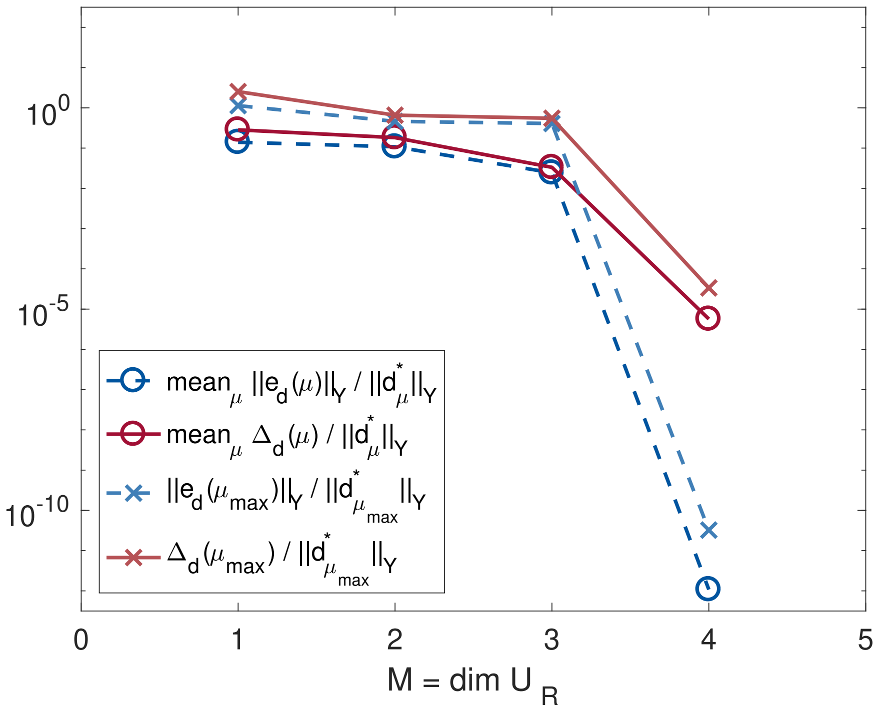
Model Correction



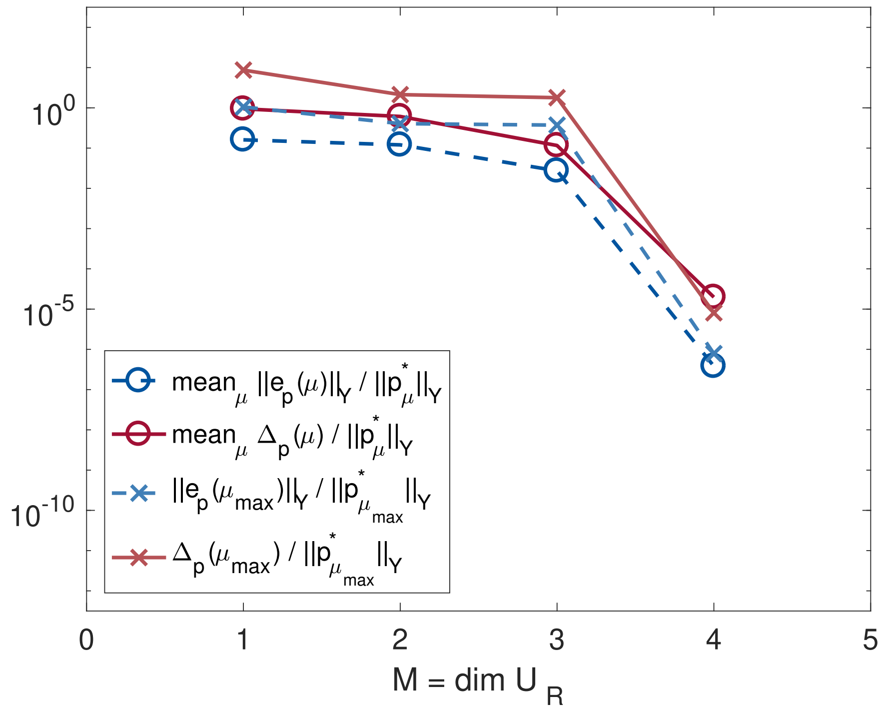
State

Numerical Results

A Posteriori Error Bounds



Observable Difference



Adjoint

200 random measurements, $\lambda = 100$.

Summary

We developed a certified RB method for 3D & 4D variational data assimilation

- model order reduction for state, adjoint, and control variables
- a posteriori bounds for error in RB approximation
- determination of unknown parameters
- estimation of model bias

Here, we focused on:

- Selection of measurements through stability-based greedy-OMP algorithm
- Reduce sensitivity to experimental noise
- Step-wise construction of RB spaces
- Application to 3D-VAR

Next steps:

- Extension to 4D-VAR
- Selection of model modifications
- Application to large-scale problems

PART III

Applications and Future Work

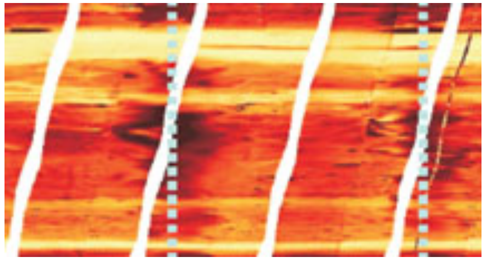
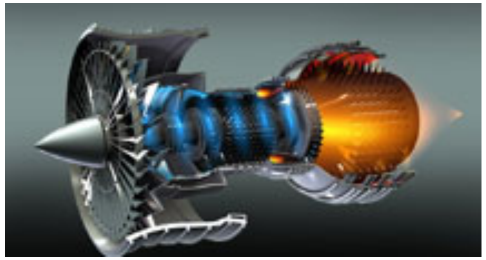
with

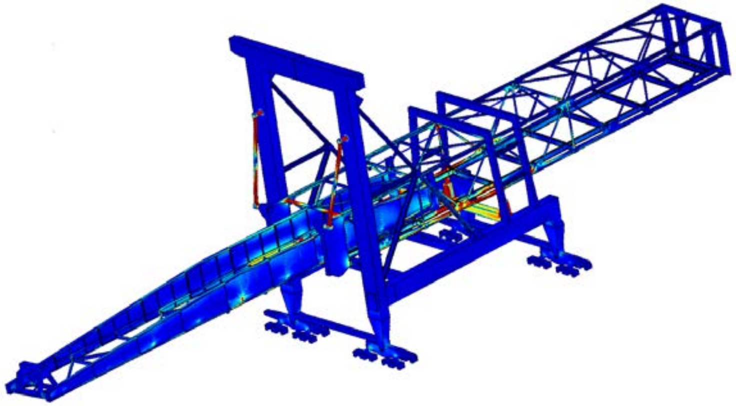
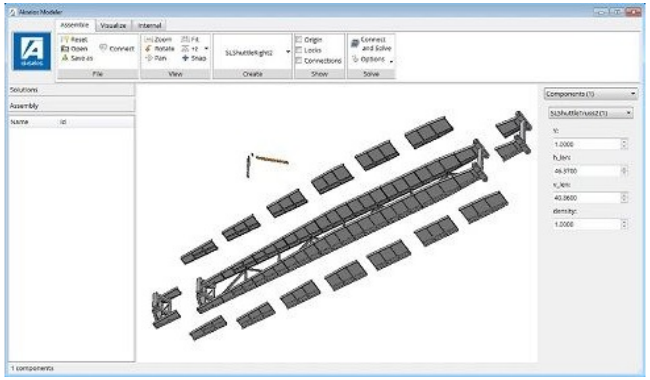
D. Degen, M. Grepl, F. Wellmann (RWTH)

M. Baragona, V. Lavezzo, R. Maessen, Z. Tokoutsi, N. Vaidya (Philips)

Industrial Applications



Source: akselos.com

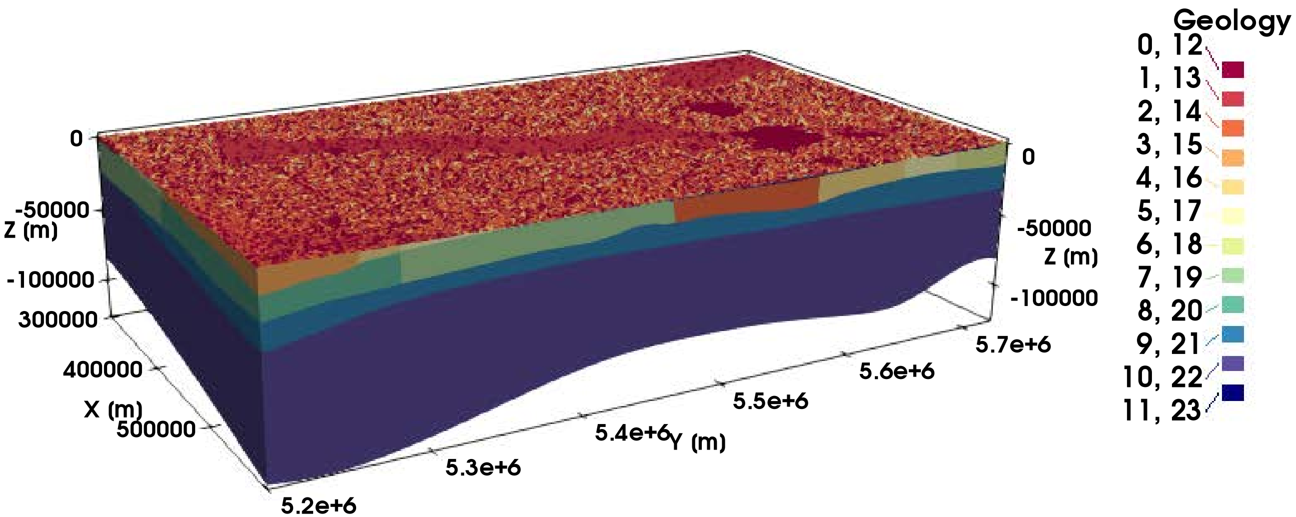
The reduced basis method is useful for the

many-query, real-time, and slim-computing contexts.

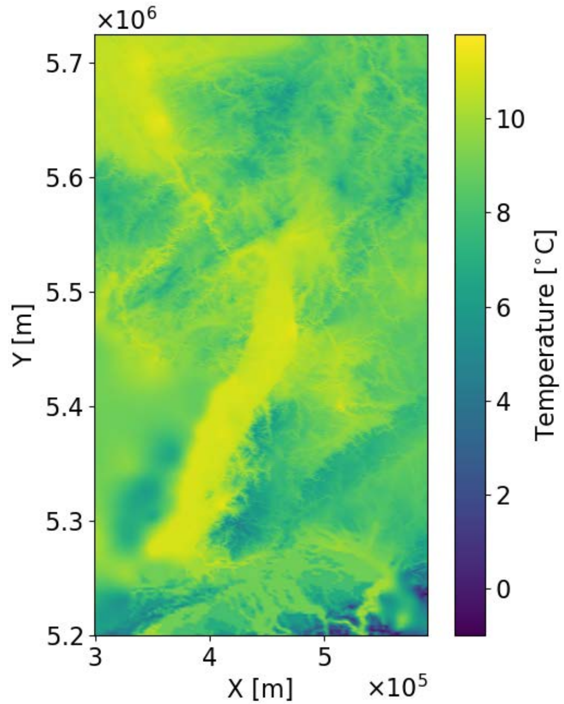
Application: Geosciences

[Degen, Wellmann, …]

Upper Rhine Graben (Germany)



Courtesy of Prof. Scheck-Wenderoth, GFZ Postdam.



Upper boundary condition

Model

Thermal diffusion with radiogenic heat production

$$\nu \nabla^2 T + S = 0$$

- Parameter Estimation
- Model Calibration
- Inverse Problems
- Sensitivity Analysis
- Data Assimilation

Acknowledgments

Collaborators:

- **M. Grepl**, IGPM, RWTH University Aachen
- **Z. Tokoutsi**, Philips Research Eindhoven
- **M. Baragona**, Philips Research Eindhoven
- **R. Maessen**, Philips Research Eindhoven

Funding:

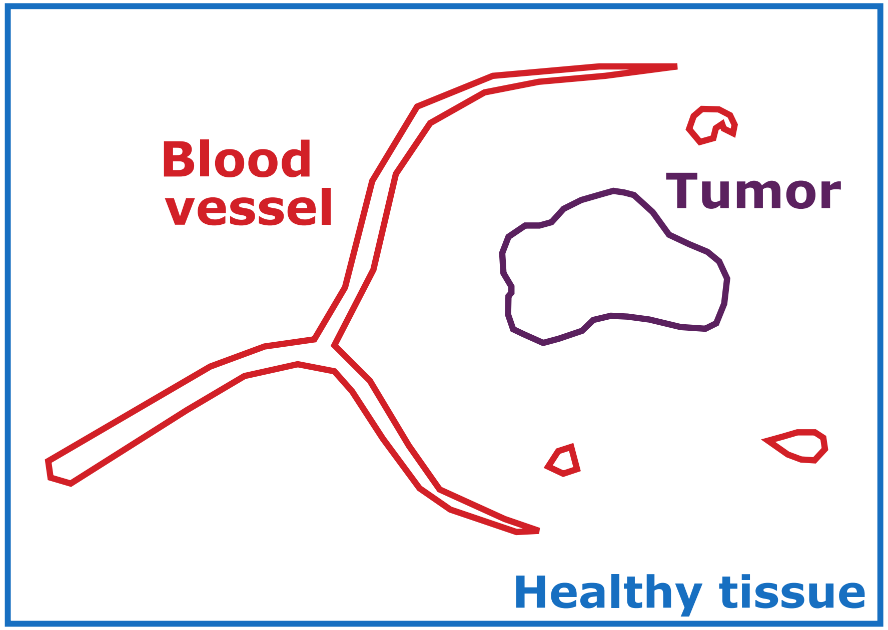
- The following work is supported by the European Commission through the Marie Sklodowska-Curie Actions (European Industrial Doctorate, Project Nr. 642445)
- NRW Fellowships für Innovationen in der Digitalen Hochschullehre

Motivation

Thermal Ablation Treatment Planning

- **Thermal Ablation:** destroy target tissue by increasing temperature above threshold.

[Chu and Dupuy , 2014]



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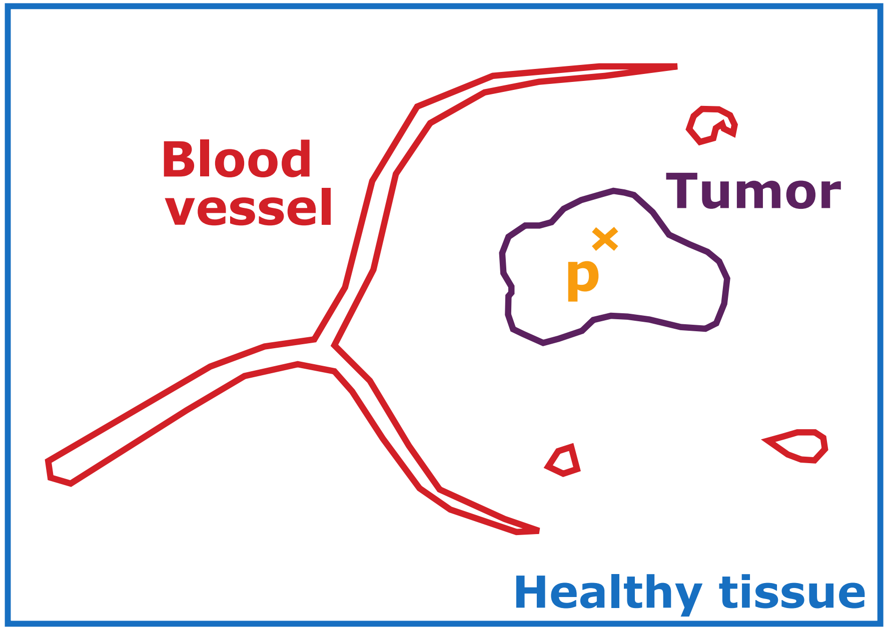
- **Treatment Planning:**
  – Determine placement parameters for ablation probes.
  – Determine device power settings.



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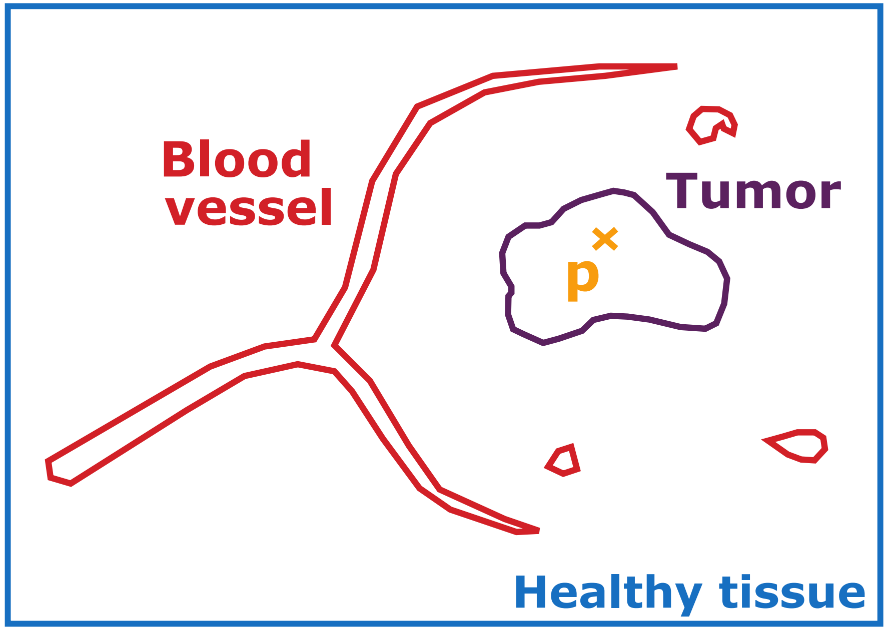

Bioheat Equation [Pennes, 1948]

Heat Diffusion in living tissue following the Pennes Bioheat model

$$
\begin{aligned}
-k\Delta T + \rho C w (T - T_{\text{core}}) &= Q, \quad && \text{in } \Omega \\
k\nabla_\nu T + h(T - T_{\text{core}}) &= 0 && \text{on } \Gamma
\end{aligned}
$$

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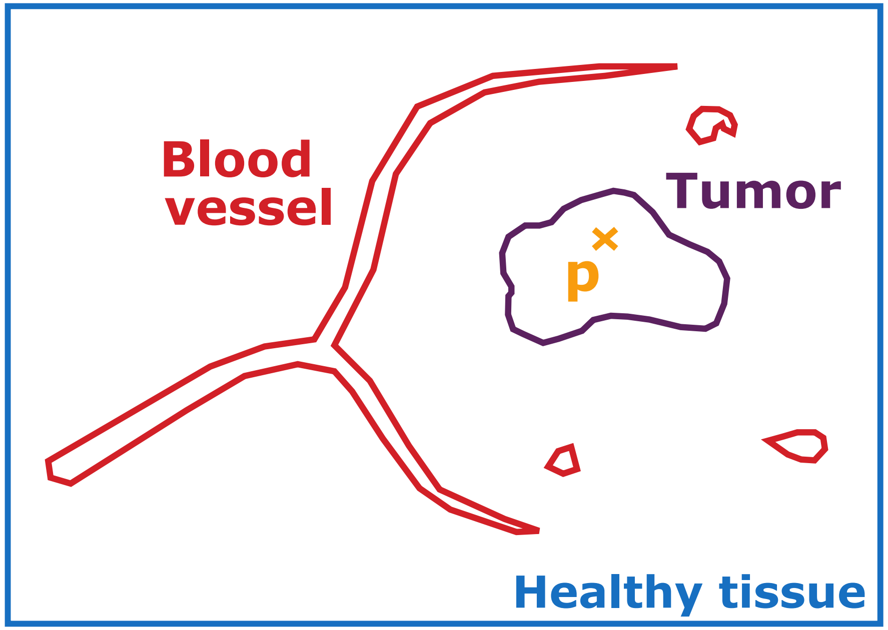
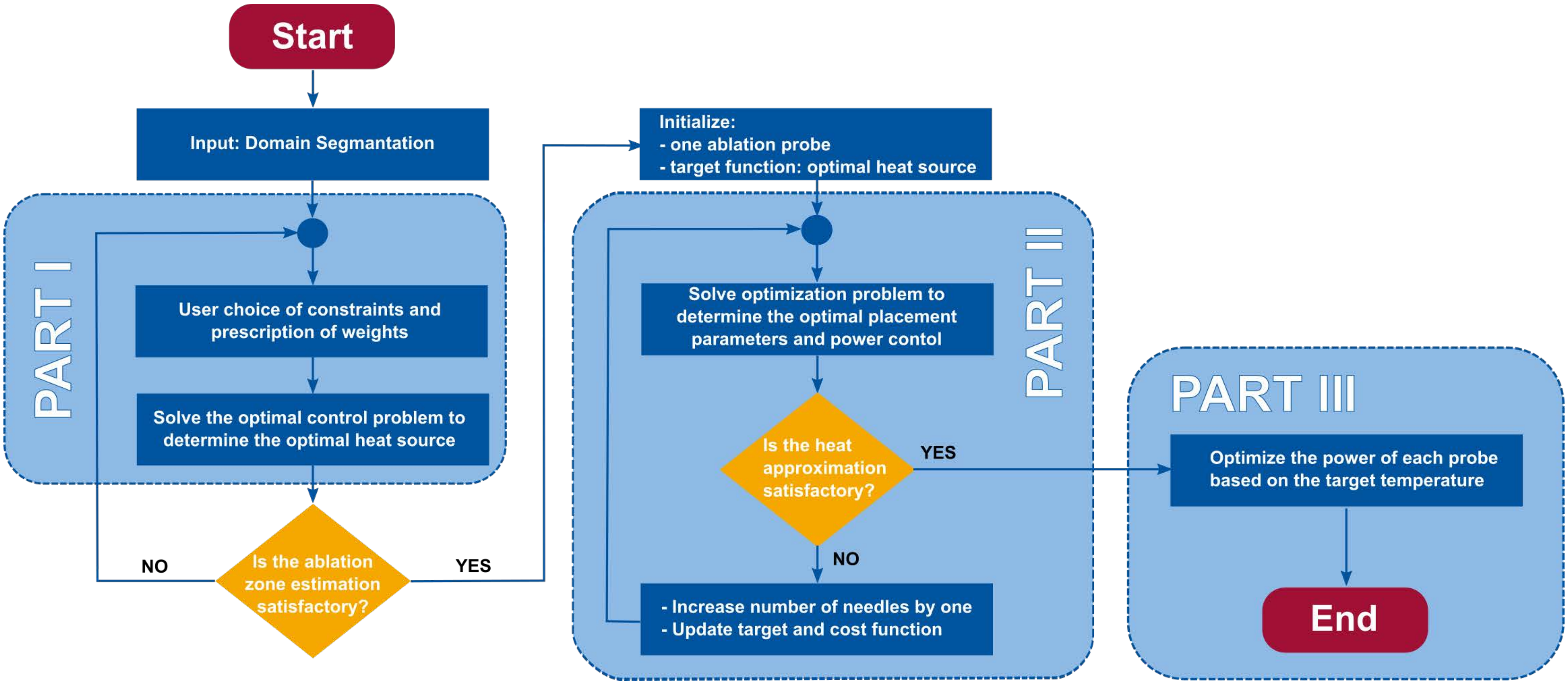


Bioheat Equation [Pennes, 1948]

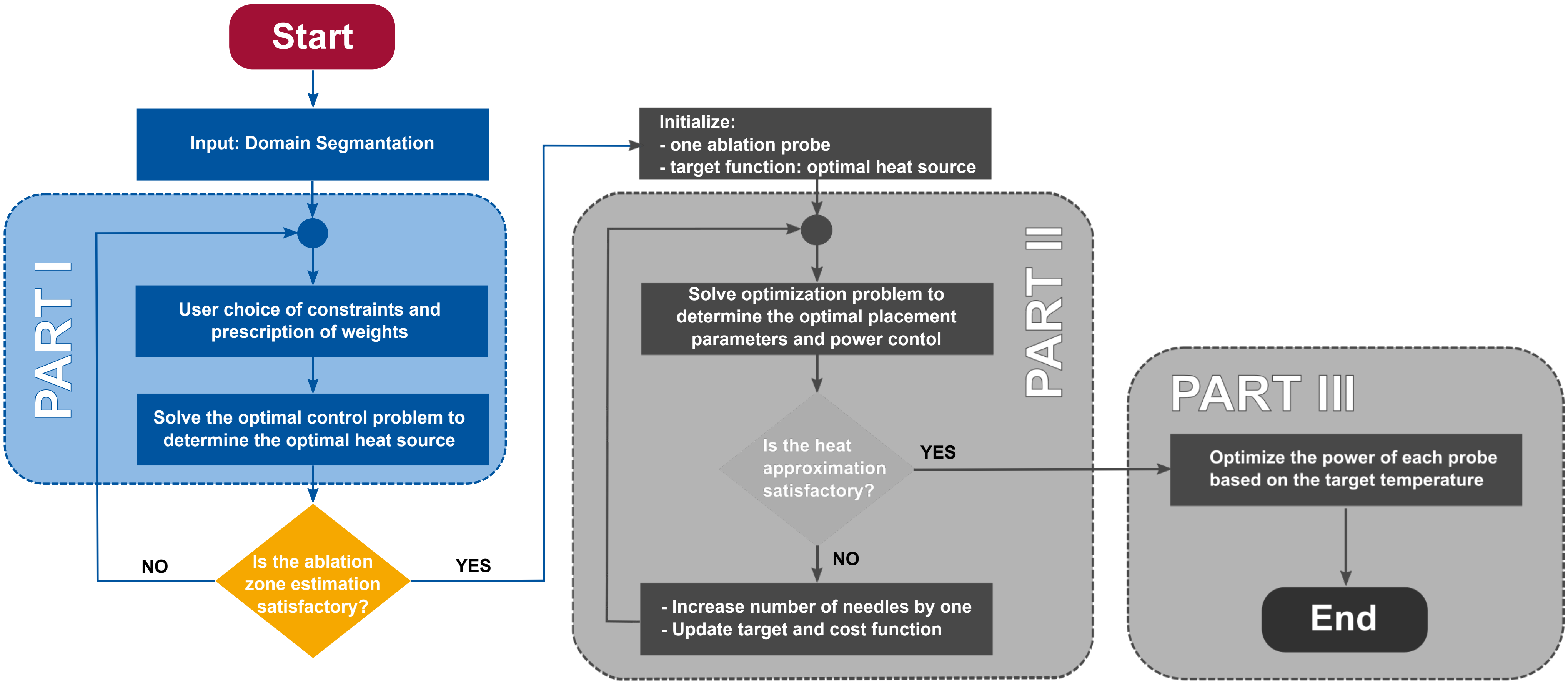
Non-dimensional Bioheat Equation

$$\begin{aligned} -k\Delta y + cy &= u, && \text{in } \Omega \\ k\nabla_\nu y + hy &= 0 && \text{on } \Gamma \end{aligned}$$

Treatment Planning Algorithm



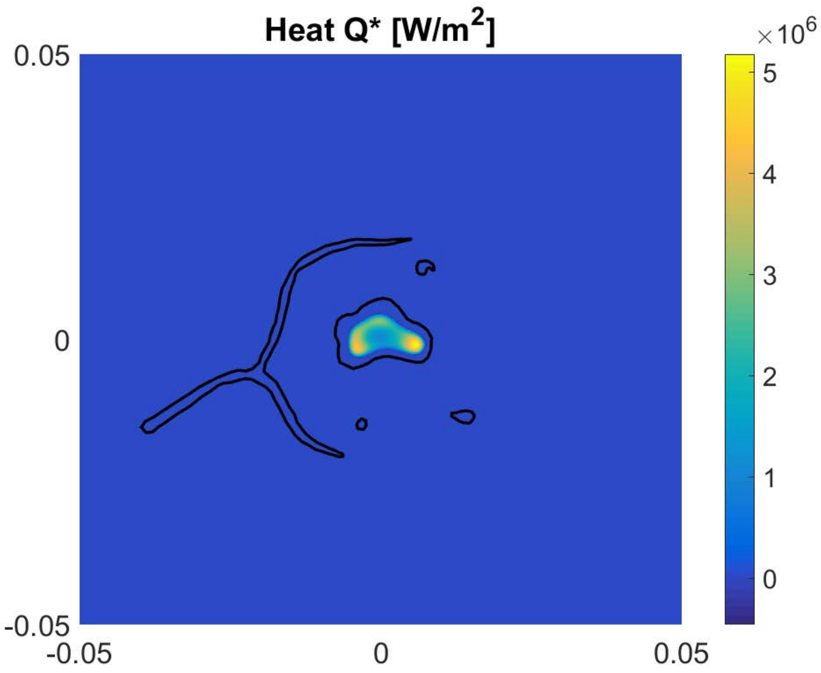
Treatment Planning Algorithm

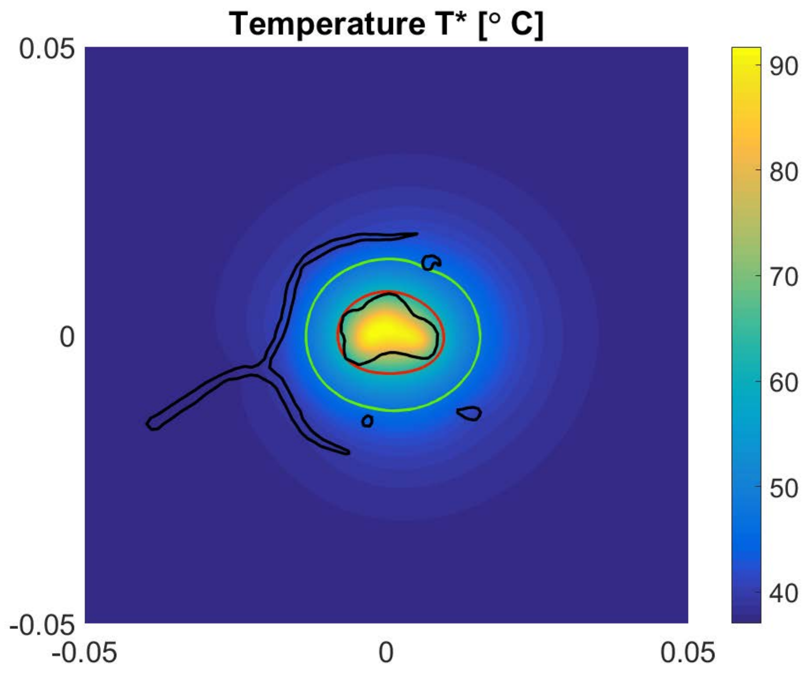


Treatment Planning Algorithm

Part I: Optimal Heat Source

$$\min_{u \in U_{ad}} J_{\text{heat}}(y, u; \mu) := \sum_{i=1}^{3} \frac{\lambda_i}{2} \|y - y_d\|^2_{L^2(\Omega_i)} + \frac{\lambda}{2} \|u\|^2_{L^2(\Omega)}$$





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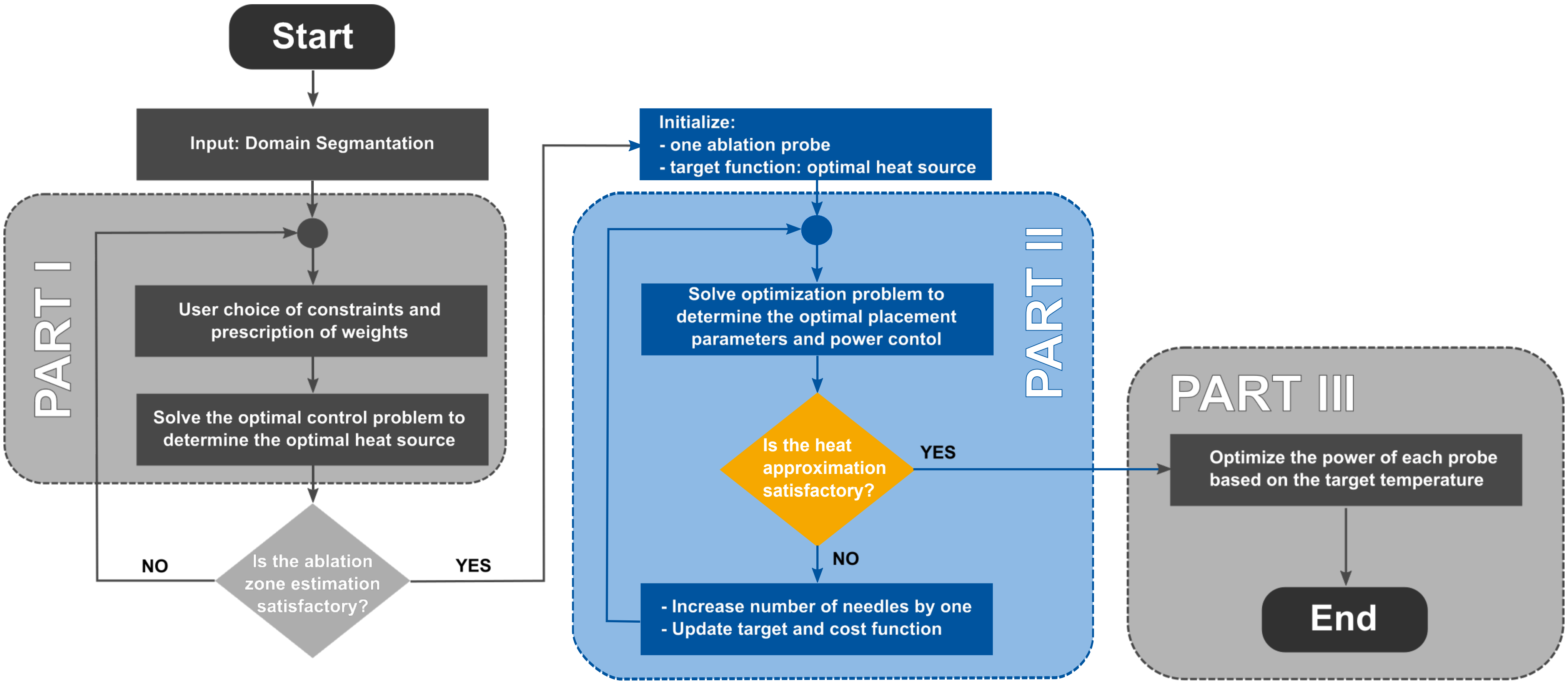
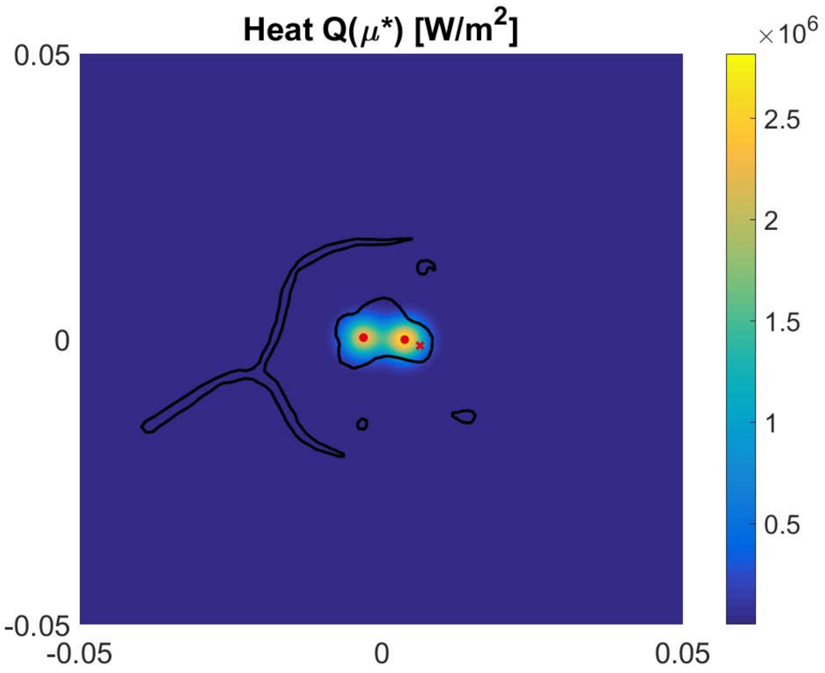
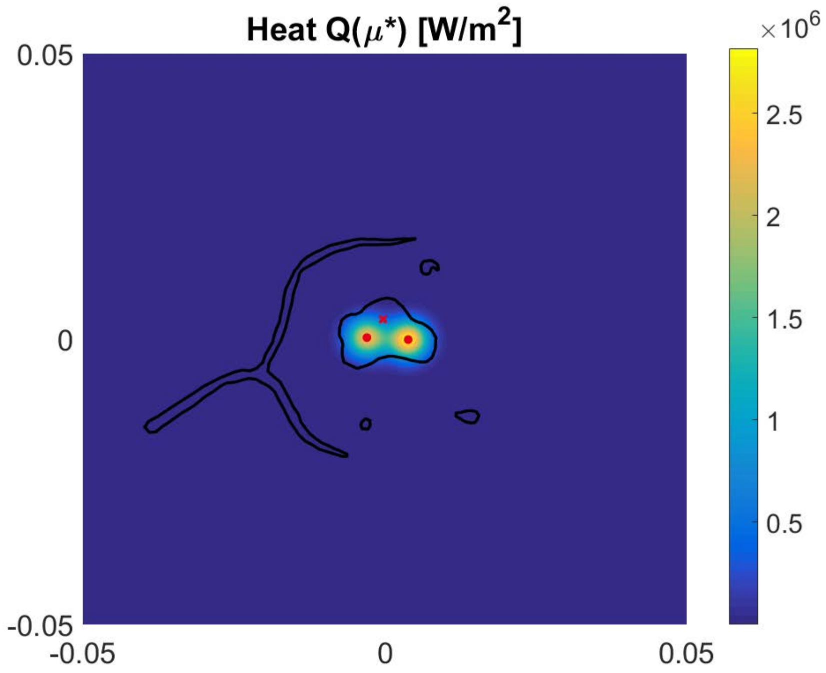


Treatment Planning Algorithm

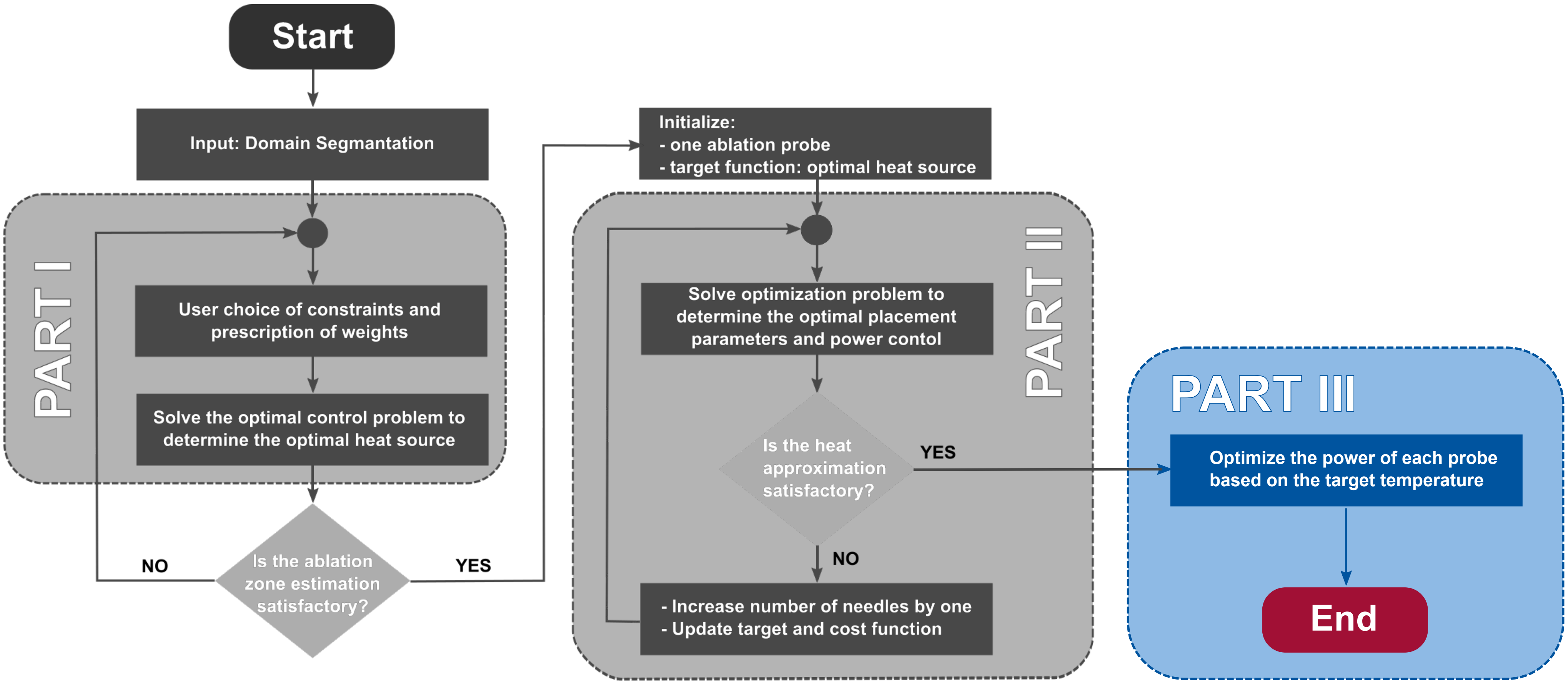
Part II: Optimize Placement and Power

$$\min_{(p,P)} J_{\text{plac}}(p,P) := \frac{1}{2}\|Q_G(x;p,P) - u^*(x)\|^2_{L^2(\Omega)}.$$





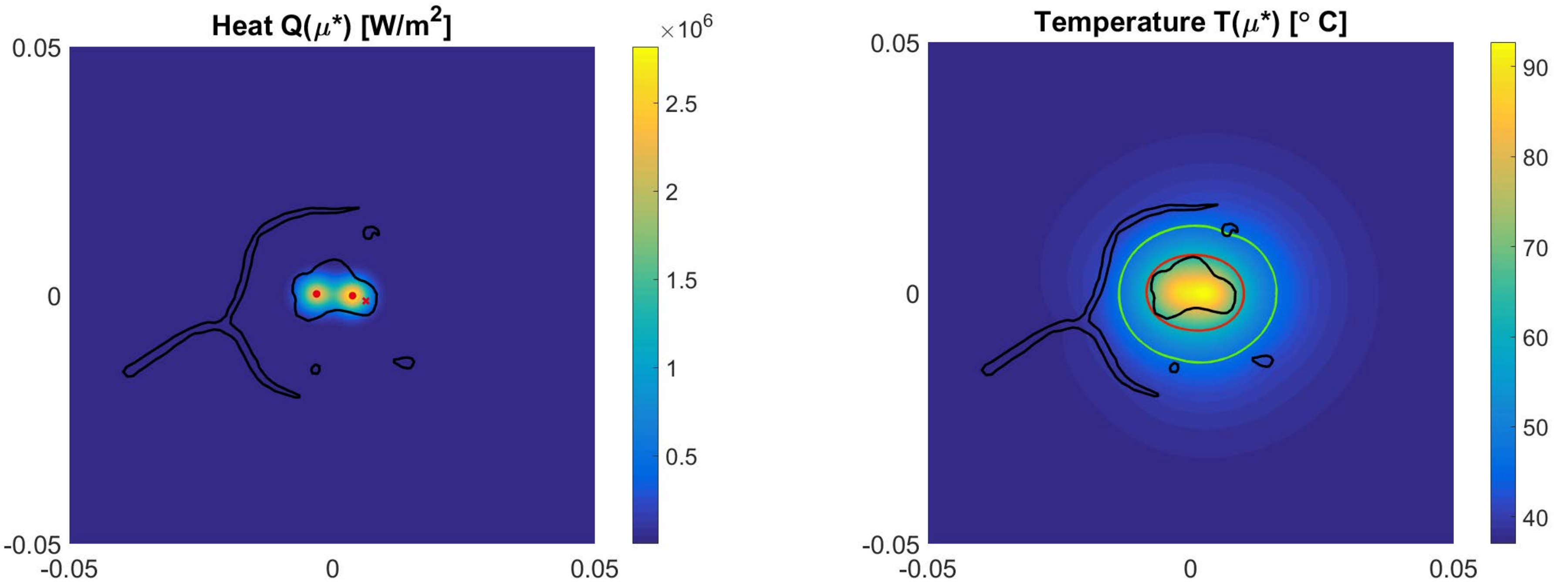
Treatment Planning Algorithm



Treatment Planning Algorithm

Part III: Power Control

$$\min_{P \geq 0} J_{\text{power}}(P_1, \cdots, P_{n_P}) := \sum_{i=1}^{3} \frac{\lambda_i}{2} \left\| y - y_d \right\|^2_{L^2(\Omega_i)}$$



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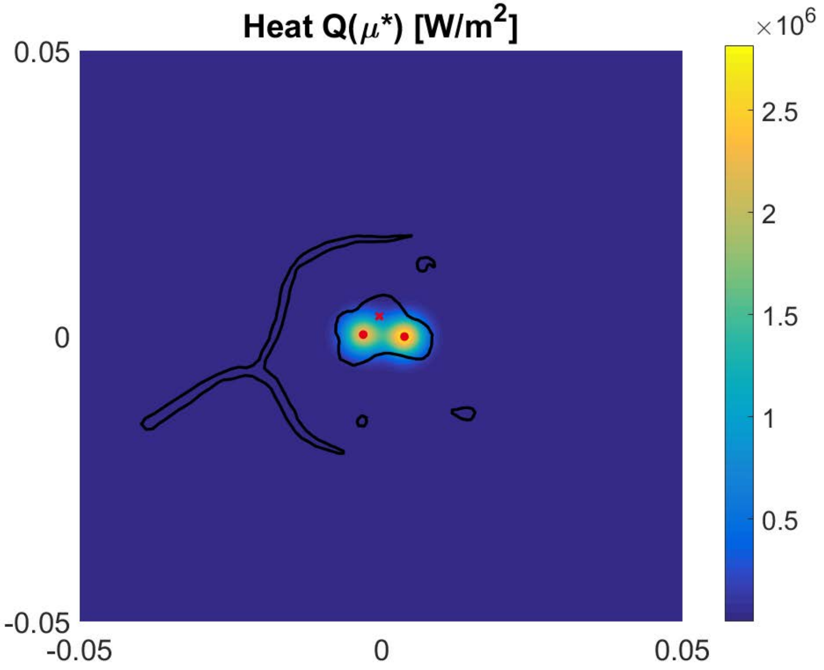

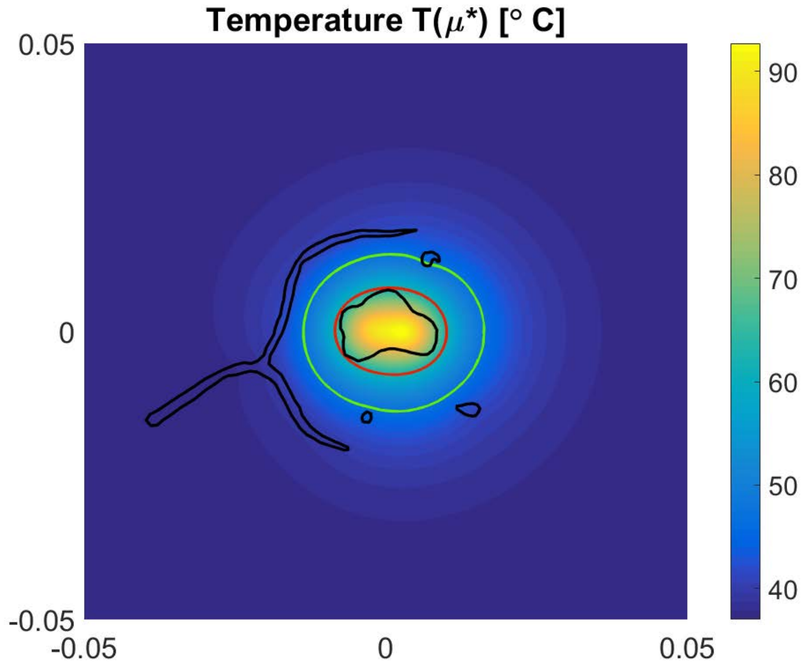

Motivation - Real Time Updates:

- Adjust regularization weights
- Adjust models with patient specific parameters
- Update solution w.r.t. geometric parameters
  - shifted tumor location
  - power control w.r.t. final probe placement

The Reduced Basis Method

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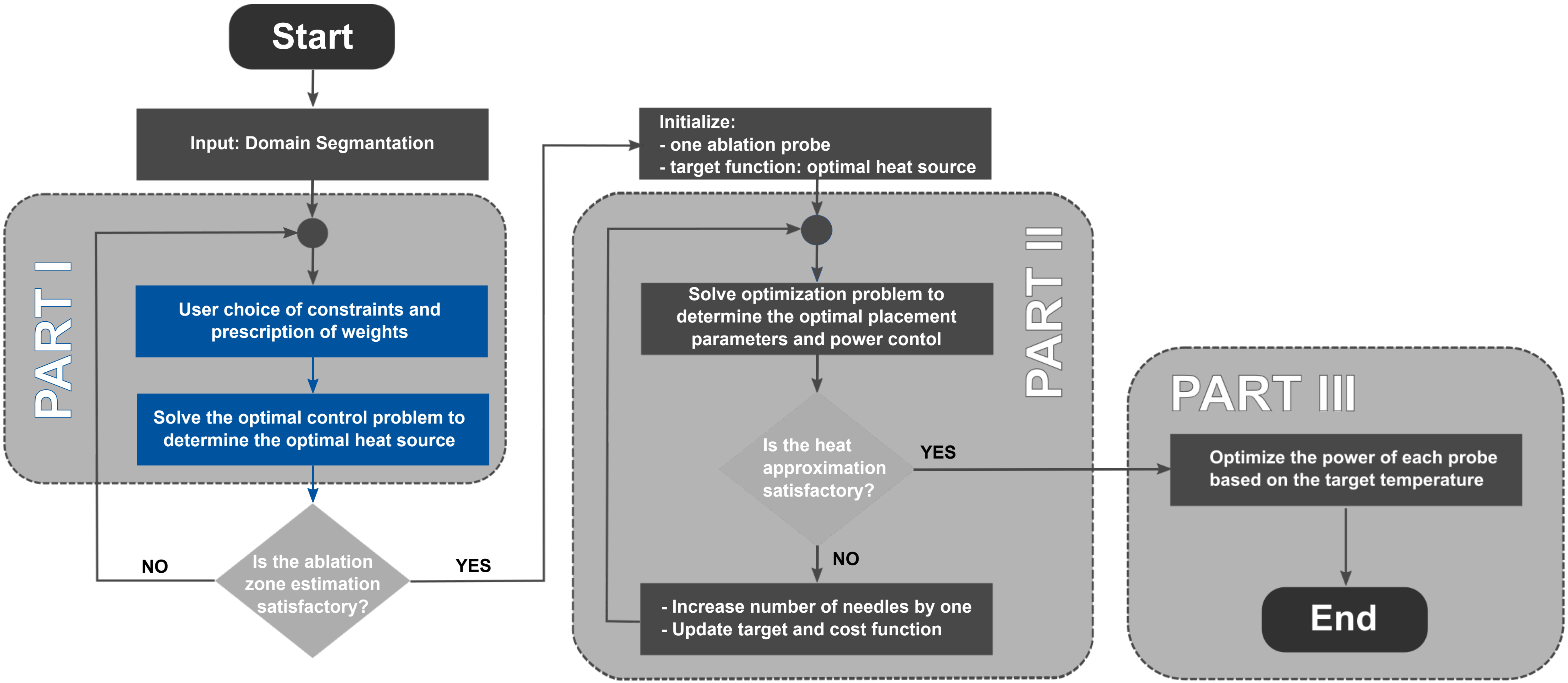
The **Reduced Basis Method** provides

- **accurate**
- **reliable**
- **efficient** surrogates
- of small dimension

- $y_N \approx y$
- $\Delta_N^y \geq \|y - y_N\|_Y$
- cost $O(N^*)$
- N small

to solutions of **parametrized PDEs** for the many query real-time contexts.

The Reduced Basis Method



Problem Set Up

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Heat Diffusion in living tissue following the Pennes Bioheat model [Pennes, 1948], [Davidson and Sherar, 2003]

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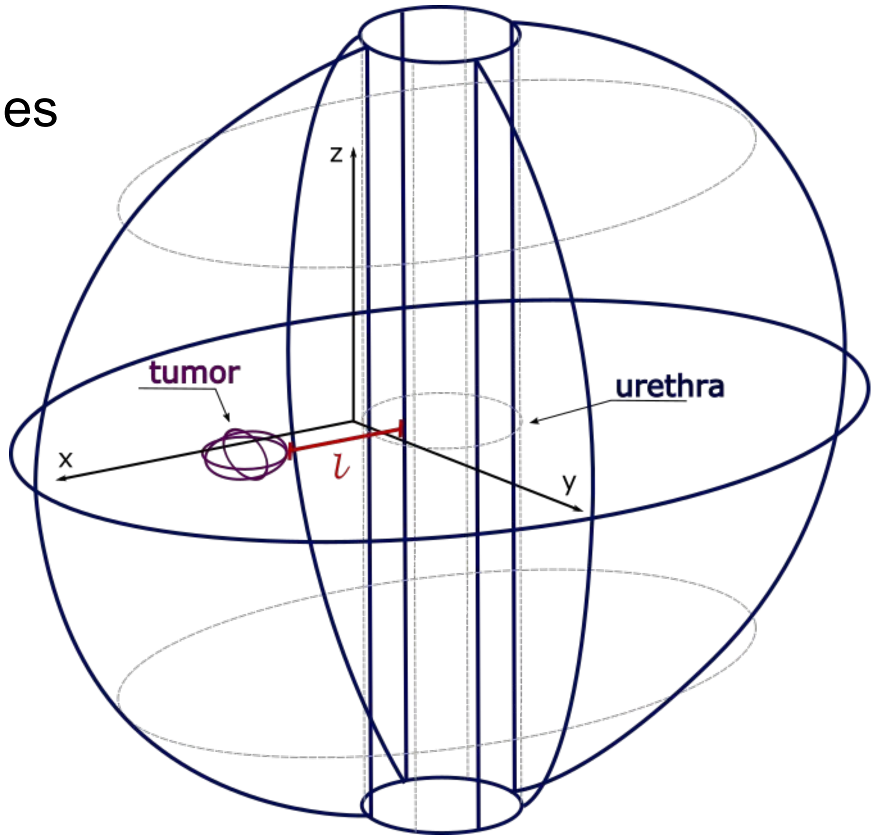
y &= 0, && \text{on } \Gamma_D
\end{aligned}
$$



Domain and mesh where created using Gmsh [Geuzaine and Remacle, 2009]

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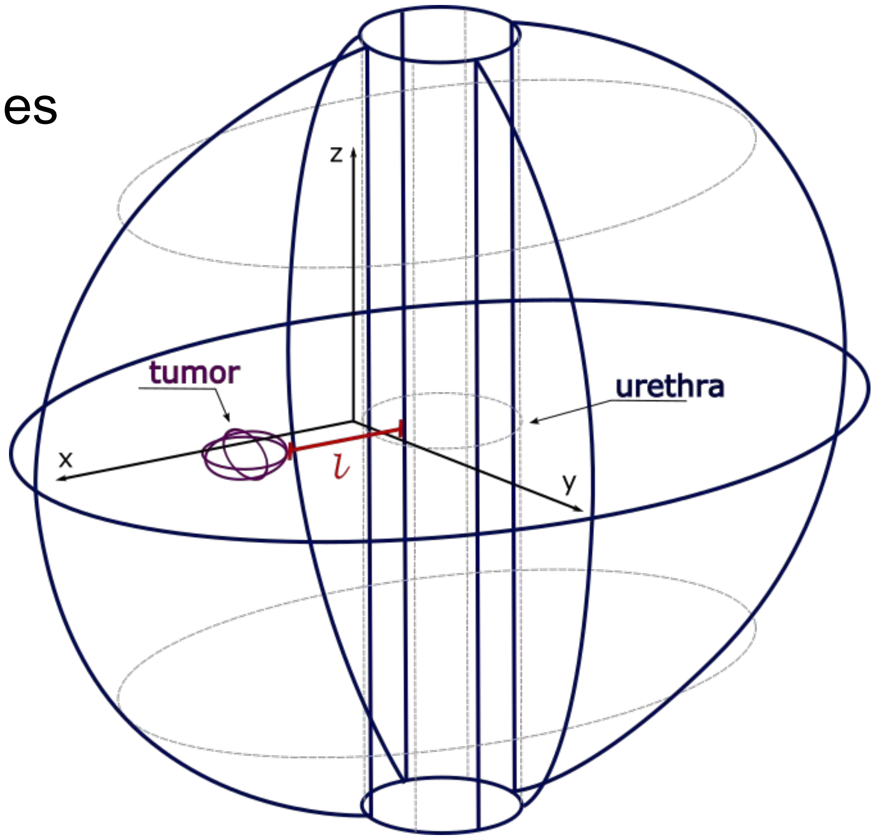
y &= 0, && \text{on } \Gamma_D
\end{aligned}
$$

Parametrization:

- Blood perfusion rate c
- Distance from urethra l
- cooling temperature y_{cool}



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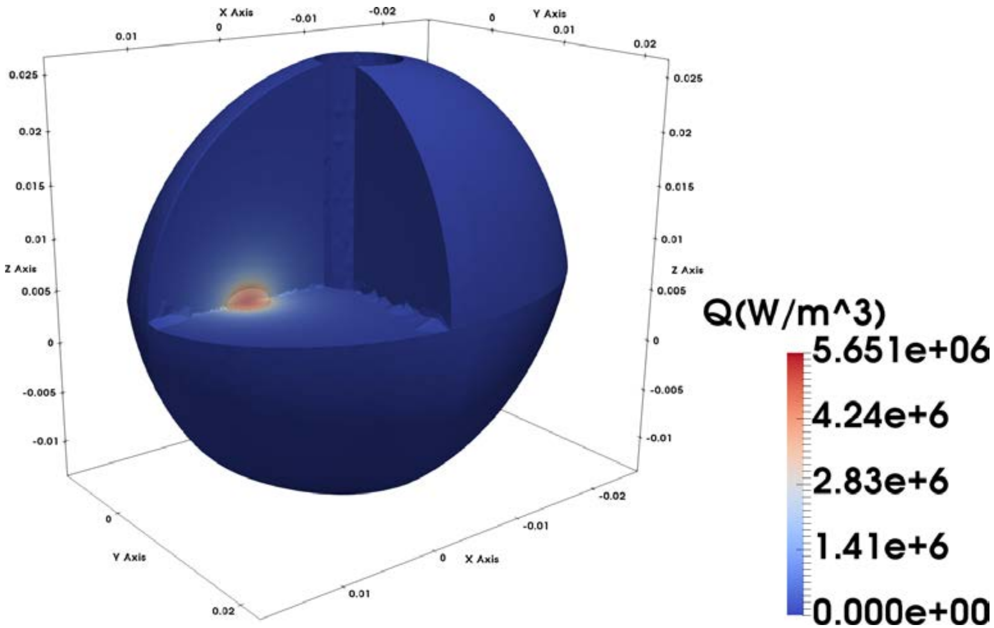
Optimal Control Problem (OCP)

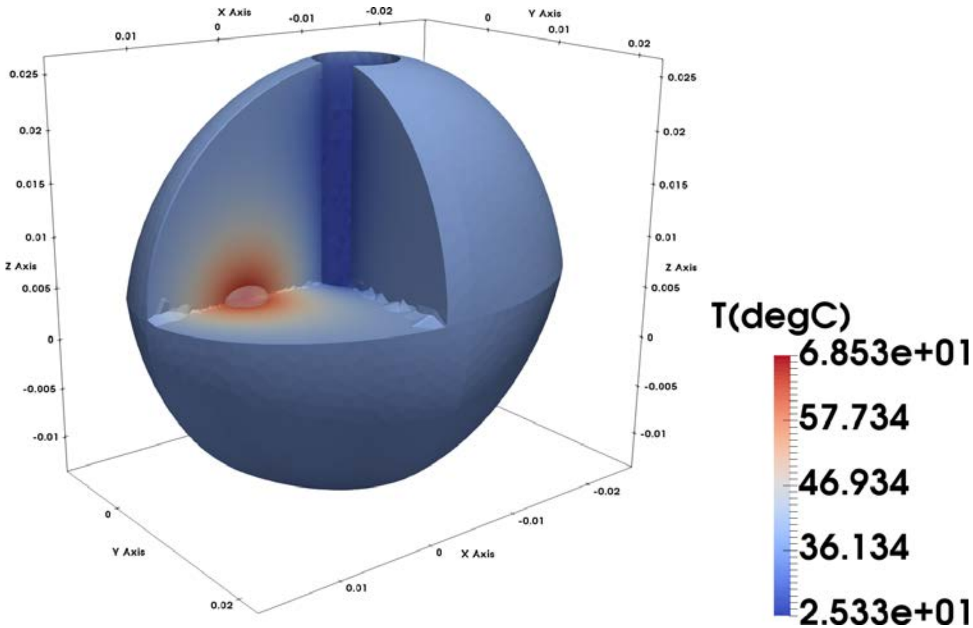
For any $\mu \in \mathcal{D}$ solve

$$\min_{y\in Y, u\in U} J_{\mathrm{heat}}(y,u;\mu) = \frac{1}{2}|y - y_d|^2_{D(\mu)} + \frac{\lambda}{2}\|u\|^2_{U(\mu)}$$

Optimal Heat u^*



Optimal Temperature y^*



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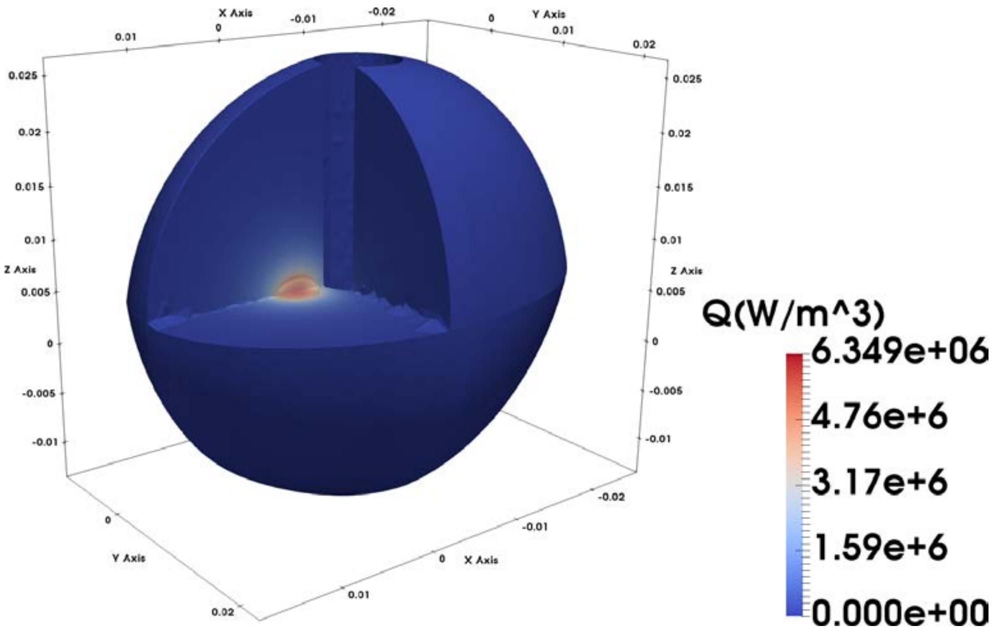

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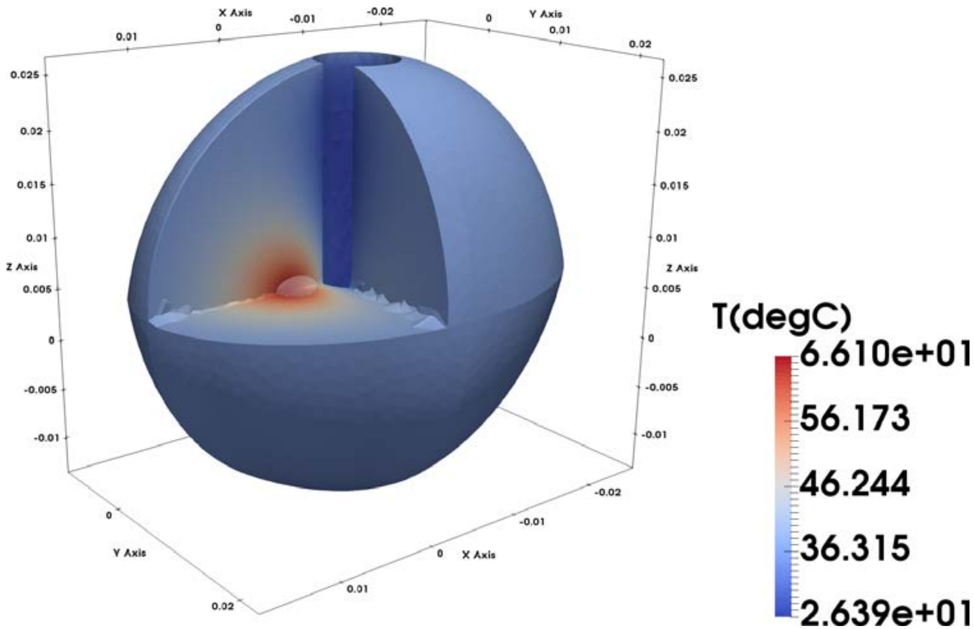
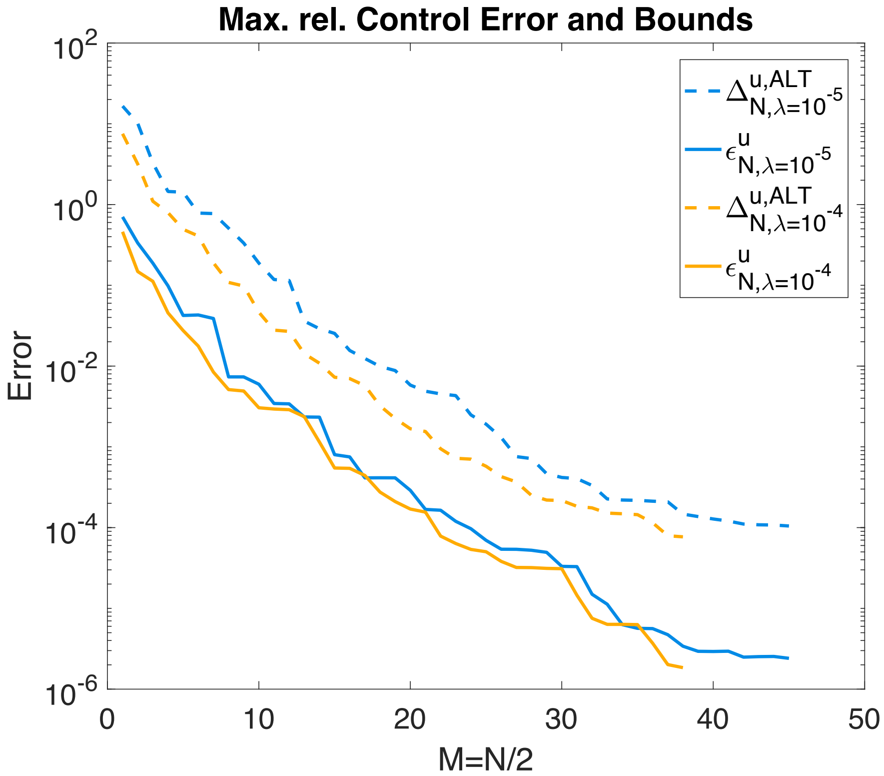
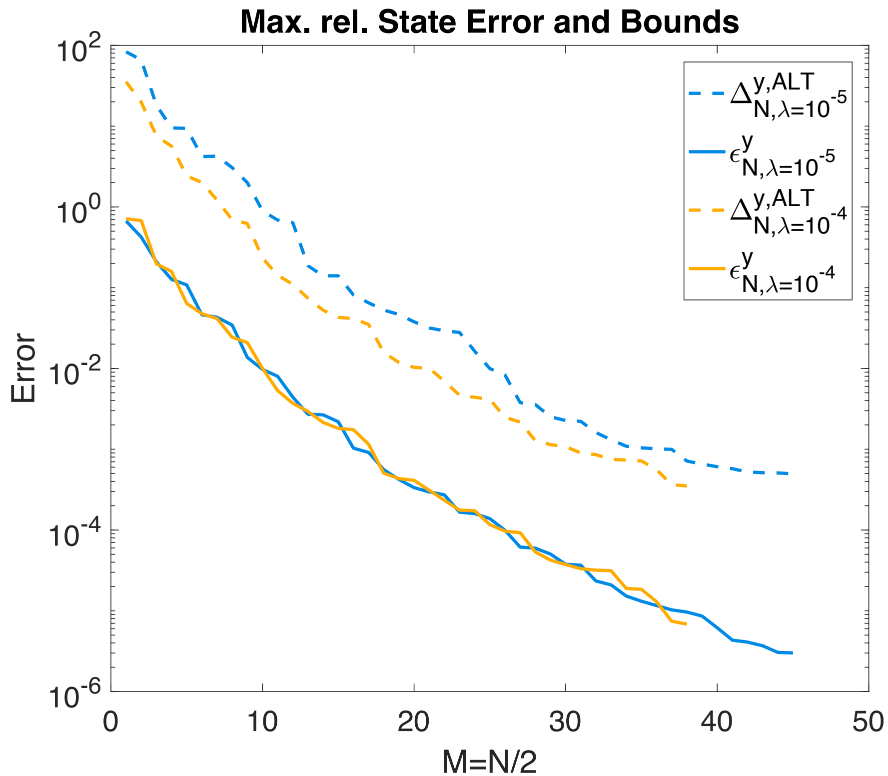


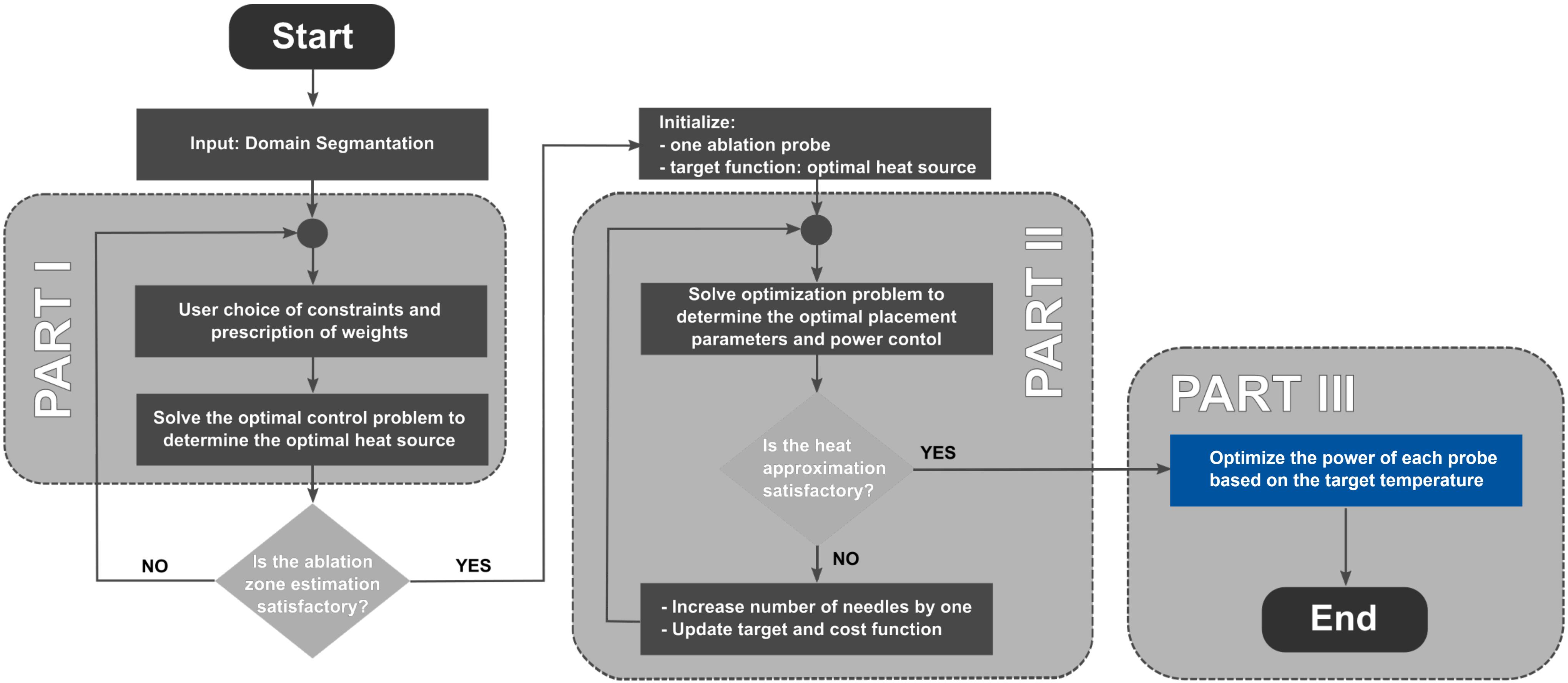
Error and Bounds **Details to appear in [T. et al., 2018]**





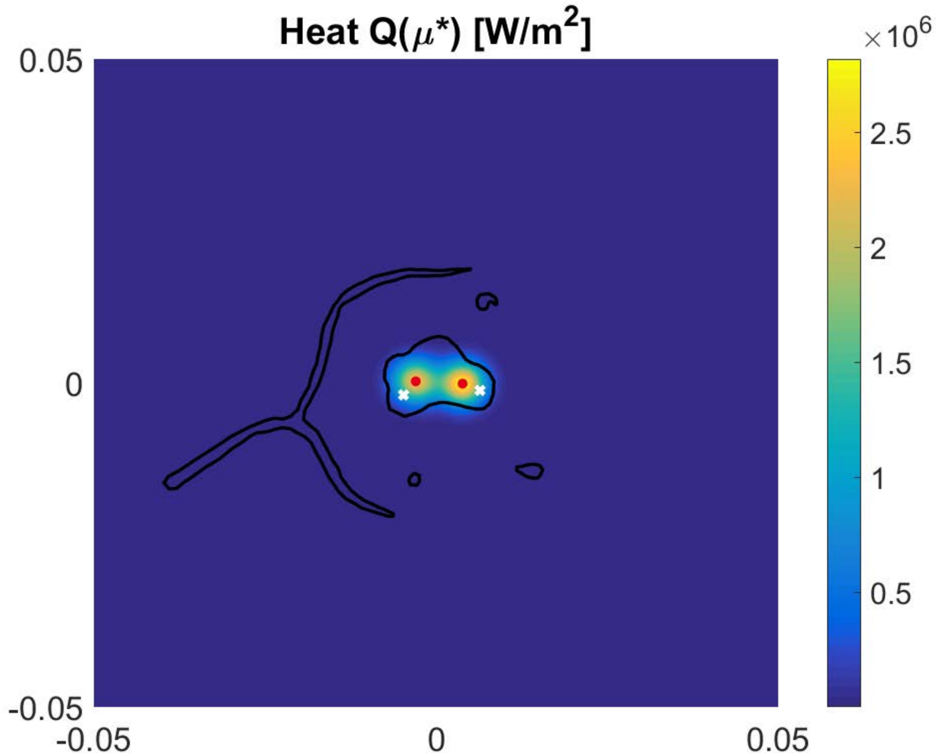
λ	FEM	RB
10^{-4}	400s	$[0.3, 1.6]$ms
10^{-5}	500s	$[0.3, 1.4]$ms

Non-Affine Problems



Motivation

Can we update the device power control in real time for different ablation probe placements?



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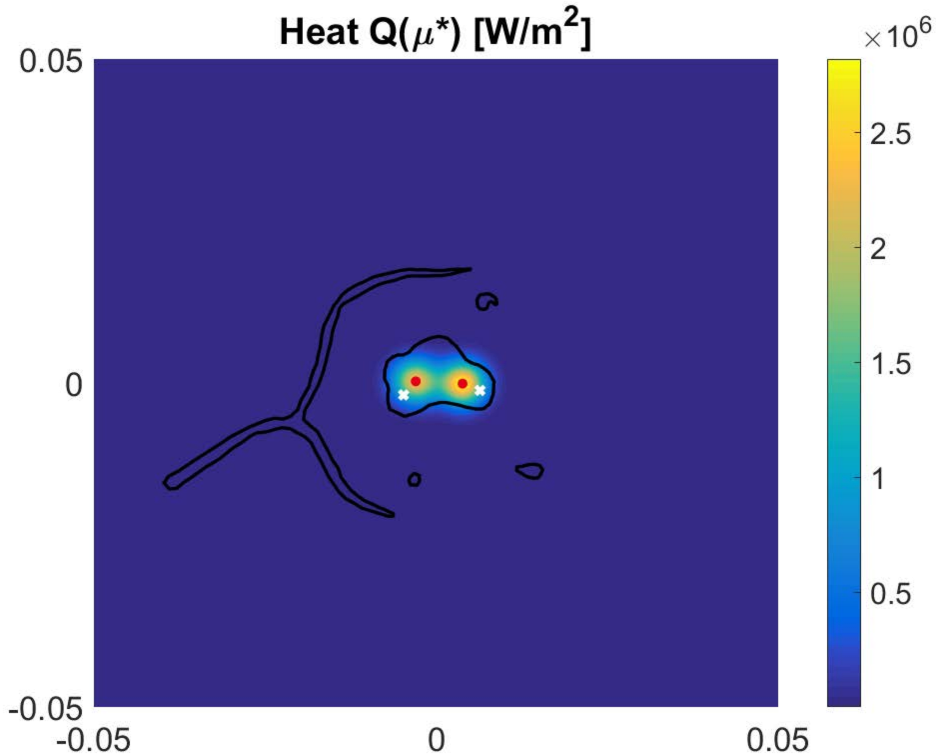

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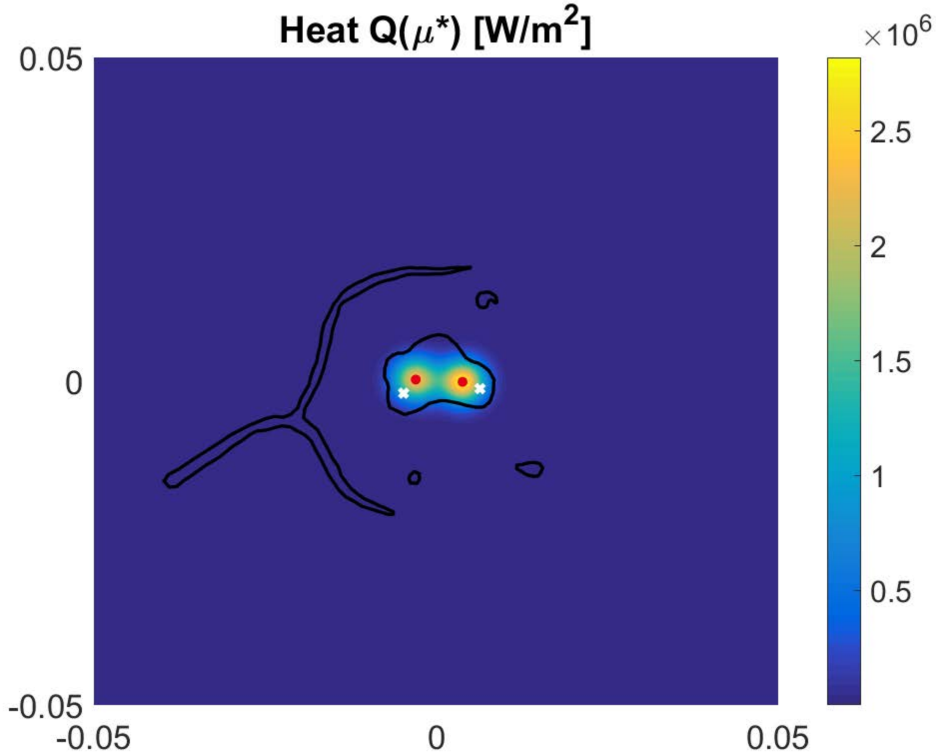


$\text{s.t.}(y, u) \in Y \times \mathbb{R}^{n_P}$ solves

$$-k\Delta y + cy = \sum_{i=1}^{n_P} P_i \, g(x; p_i), \qquad \text{in } \Omega$$

$$k\nabla_\nu y + hy = 0, \qquad \text{on } \Gamma$$

Non-Affine Problems

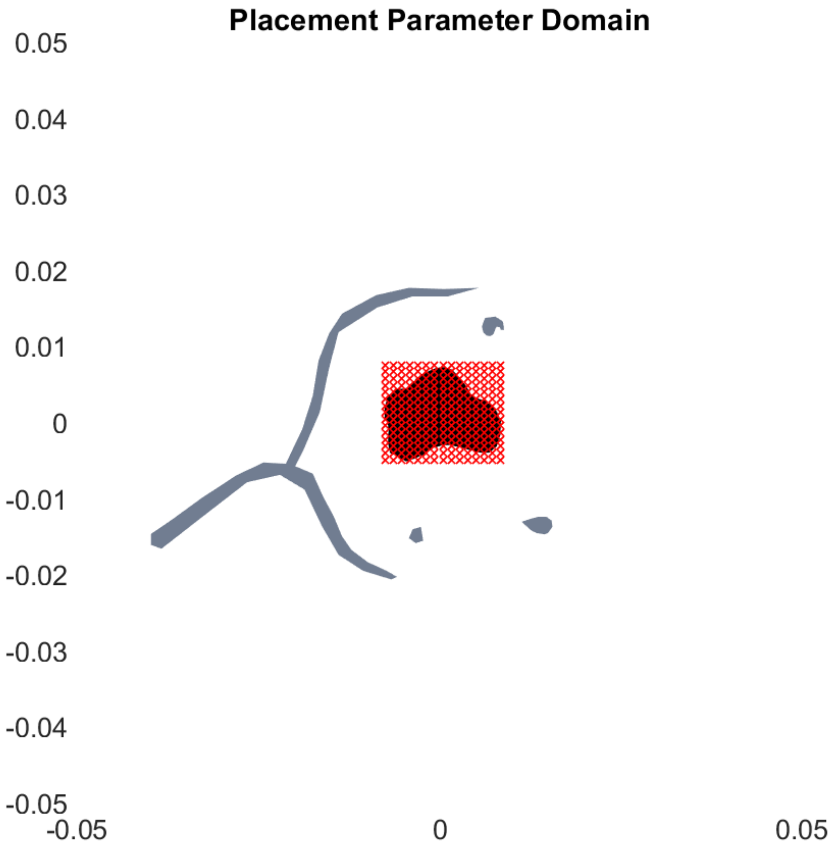
EIM [Barrault, Maday, Nguyen, Patera, 2004]

- Use EIM to construct collateral basis

$$W_M^g := \text{span}\{\hat{g}^1 = g(\mu_1), \cdots, \hat{g}^M = g(\mu_M)\}$$

- Affinely decomposable approximation

$$g(.;\mu) \approx g_M(.,\mu) = \sum_{m=1}^{M} \omega_m(\mu)\hat{g}^m(x).$$



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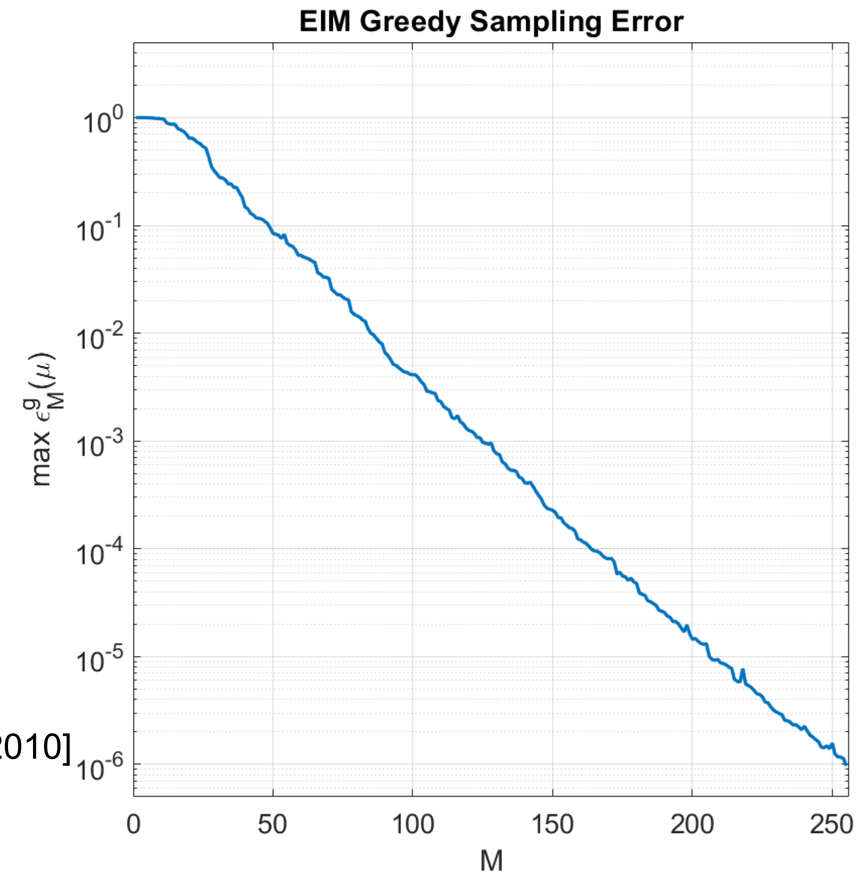
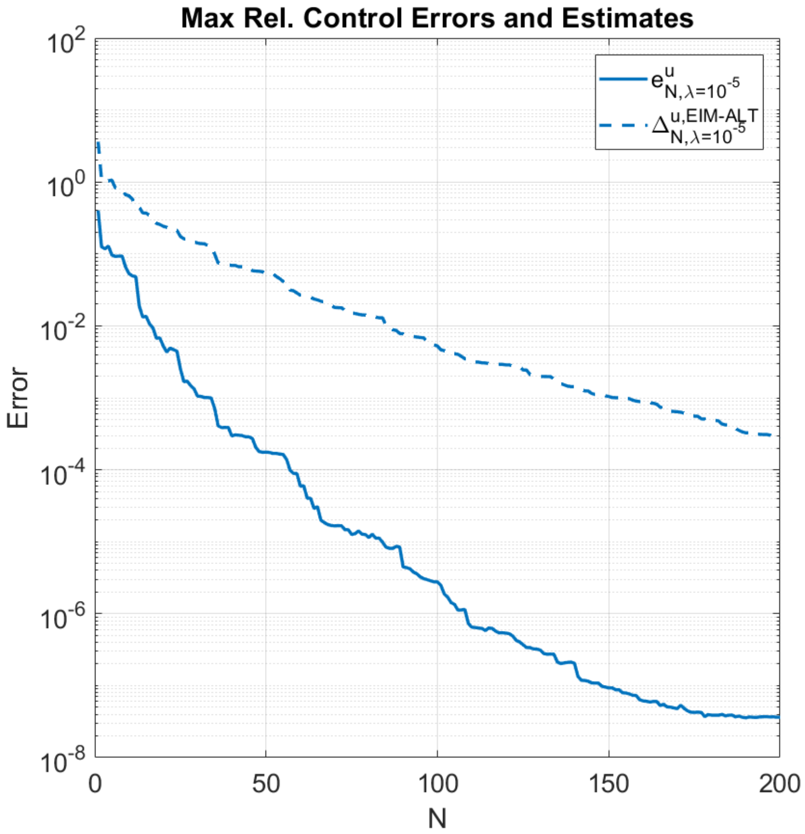
- Estimate interpolation error [Eftang, Grepl, Patera , 2010]

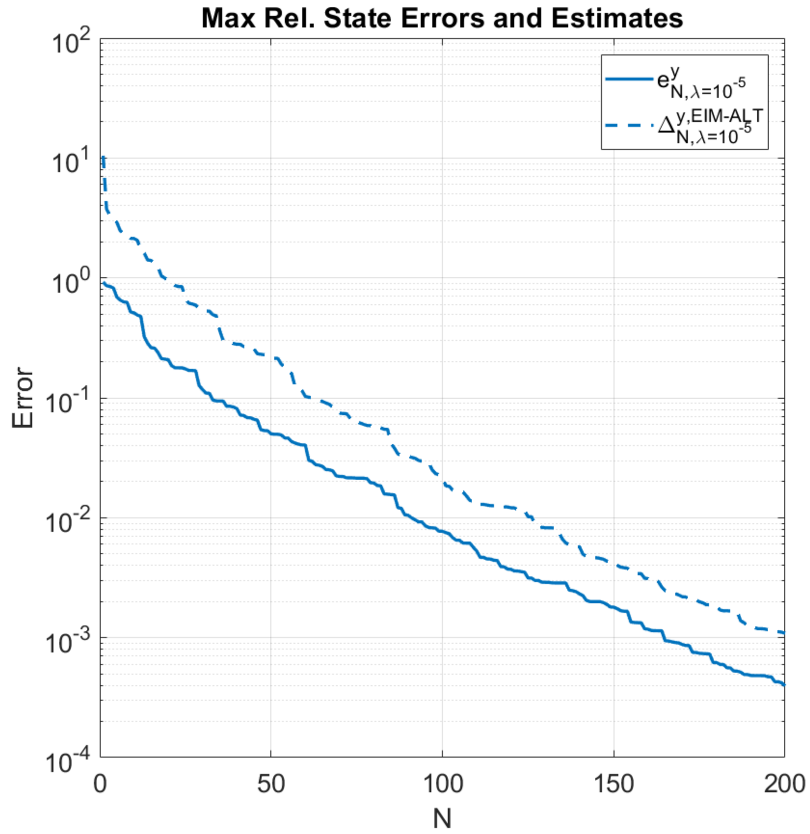
$$\varepsilon_M^g(\mu) := \|g(.;\mu) - g_M(.;\mu)\|_{L^\infty(\Omega)} \leq \hat{\varepsilon}_M^g(\mu)$$



Non-Affine Problems

Relative Errors and Error Estimates





EIM tol	M	FE time	RB time
$1e-6$	256	1.1 s	0.1 – 10 ms

Outlook and Conclusions

Overview:

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Ongoing Work:

- Apply our work to model reduction for time dependent power control.

Outlook and Conclusions

Literature

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Discussion

Questions or comments?

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