Reduced Basis Methods:
From Key Ingredients to 4DVar

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Acknowledgments

Collaborators:

- Sébastien Boyaval
- Mark Kärcher
- Karen Veroy

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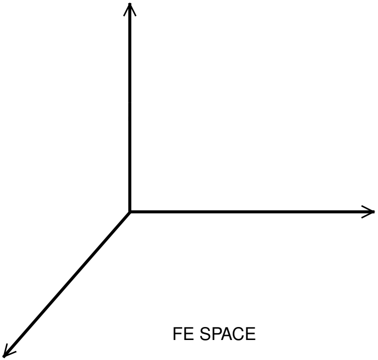
Part I

A Reduced Basis Primer

The Reduced Basis Method



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

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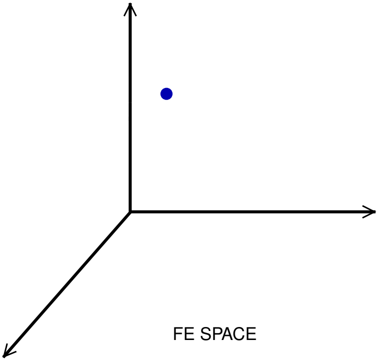

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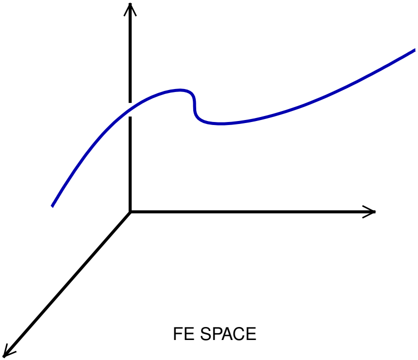

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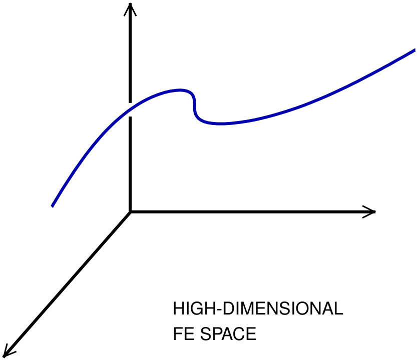

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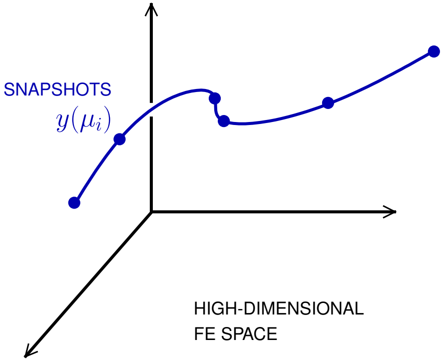
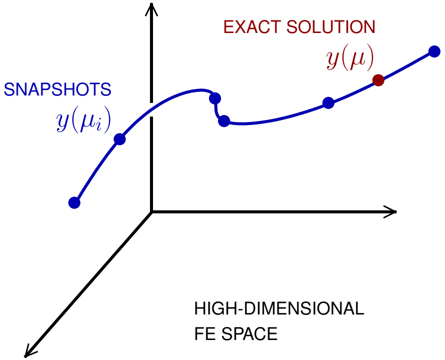


$$Y_N = \text{span}\{\, y(\mu_i)\,,\; i = 1, \dots, N \,\}$$

The Reduced Basis Method



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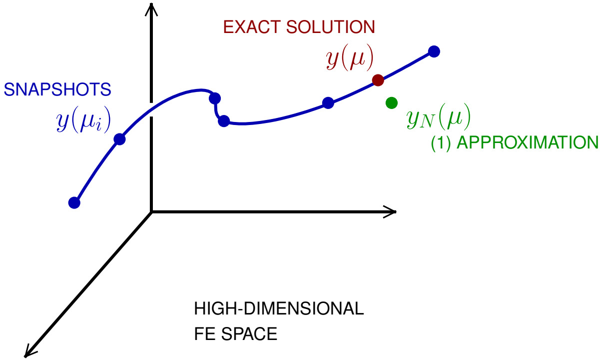
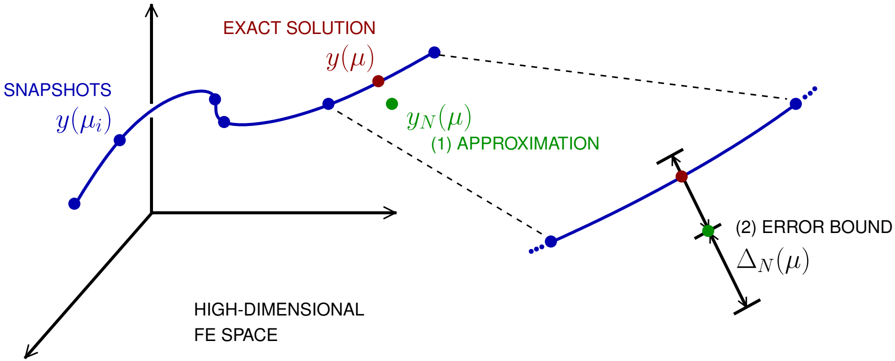


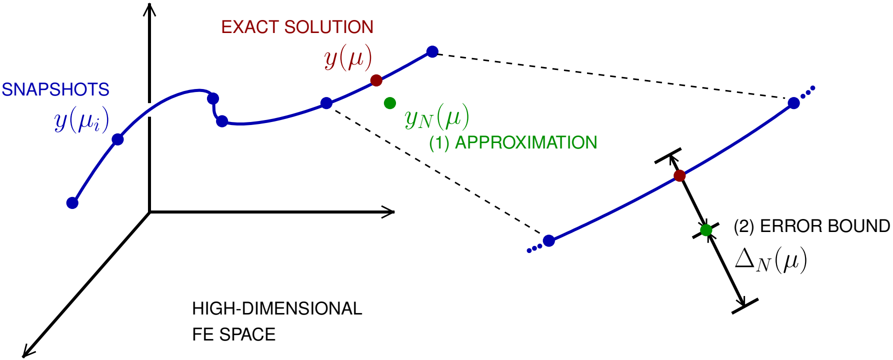
$$a(y_N(\mu), v; \mu) = f(v; \mu), \quad \text{for all } v \in Y_N.$$

The Reduced Basis Method



$$\|y(\mu) - y_N(\mu)\|_Y \;\leq\; \Delta_N^y(\mu) \;:=\; \frac{\|r_N(\cdot;\mu)\|_{Y'}}{\alpha_{LB}(\mu)}$$

The Reduced Basis Method



(3) OFFLINE-ONLINE COMPUTATIONAL DECOMPOSITION

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

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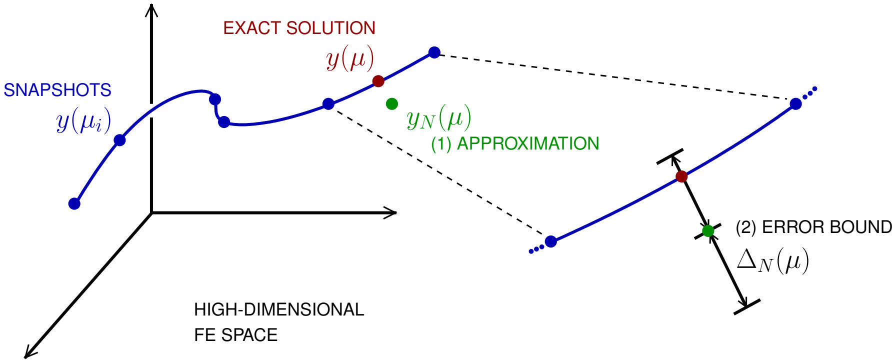

(3) OFFLINE-ONLINE COMPUTATIONAL DECOMPOSITION

(4) GREEDY ALGORITHM

$$\boldsymbol{\mu_{n+1} = \arg\max_{\mu \in \mathcal{D}_s} \frac{\Delta_n^y(\mu)}{\|y_N(\mu)\|_Y}}$$

Problem Statement

Given $\underbrace{\boldsymbol{\mu}}_{\text{PARAMETER}} \in \underbrace{\mathcal{D}}_{\substack{\text{PARAMETER}\\ \text{DOMAIN}}},$

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Given $\underbrace{\mu}_{\text{PARAMETER}} \in \underbrace{\mathcal{D}}_{\text{PARAMETER DOMAIN}}$, evaluate

$$s(\mu) = \ell(y(\mu); \mu) \qquad \text{OUTPUT}$$

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where $\underbrace{y(\mu)}_{\text{FIELD VARIABLE}} \in \underbrace{Y}_{\text{FE SPACE}}$ satisfies

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

and

$f(v; \mu),\ \ell(v; \mu)$ are bounded linear functionals

$a(\cdot, \cdot; \mu) : Y \times Y \to \mathbb{R}$ is continuous and coercive

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

Problem Statement (Algebraic Formulation)

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

$$\underbrace{s(\mu)}_{\text{OUTPUT}} = \underbrace{L(\mu)^T}_{\substack{\text{OUTPUT} \\ \text{VECTOR}}} \underline{y}(\mu)$$

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Difficulties:

- Need to solve $\text{PDE}_{\mathcal{N}}(\mu)$ numerous times at different values of μ
- Finite element space Y has large dimension $\mathcal{N}$

(1) Approximation

We let

$$\boldsymbol{Y_N} = \textbf{span}\{\ \underbrace{\boldsymbol{y}(\boldsymbol{\mu_i})}_{\text{SNAPSHOTS}}\ ,\ \boldsymbol{i} = \mathbf{1}, \ldots, \boldsymbol{N}\ \}$$

and compute our approximation as

$$\boldsymbol{s_N}(\boldsymbol{\mu}) = \boldsymbol{\ell}(\boldsymbol{y_N}(\boldsymbol{\mu}); \boldsymbol{\mu})$$

where $\boldsymbol{y_N}(\boldsymbol{\mu}) \in \boldsymbol{Y_N}$ satisfies

$$\boldsymbol{a}(\boldsymbol{y_N}, \boldsymbol{v}; \boldsymbol{\mu}) = \boldsymbol{f}(\boldsymbol{v}; \boldsymbol{\mu}), \quad \text{for all } \boldsymbol{v} \in \boldsymbol{Y_N}. \qquad \text{ROM}_{\boldsymbol{N}}(\boldsymbol{\mu})$$

(1) Approximation (Algebraic Formulation)

We let

$$Z_N = [\ \underbrace{\zeta_1}\ \ \underbrace{\zeta_2}\ \ \cdots\ \ \underbrace{\zeta_N}\ ] \quad \text{s.t.} \quad y_N(\mu) = Z_N \underline{\mathrm{y}}_N(\mu)$$

Y-ORTHONORMAL SNAPSHOTS ζ_i "$=$" $y(\mu_i)$

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where $\underline{y}_N(\mu) \in \mathbb{R}^N$ satisfies

$$\underbrace{Z_N^T A(\mu) Z_N}_{\mathbf{A}_N(\mu)}\ \underline{y}_N(\mu) = \underbrace{Z_N^T F(\mu)}_{\mathbf{F}_N(\mu)}$$

$$\mathbf{A}_N(\mu)\ \underline{y}_N(\mu) = \mathbf{F}_N(\mu)$$

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How do we quantify the error?

(2) Error Estimation

Let $\alpha(\mu)$ be the **coercivity constant** of a

$$\alpha(\mu) := \inf_{v \in Y} \frac{a(v, v; \mu)}{\|v\|_Y^2}$$

and define **residual** $r_N(v; \mu) := f(v; \mu) - a(y_N, v; \mu), \; \forall v \in Y$.

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The **error**, $e_N(\mu) := y(\mu) - y_N(\mu)$, then satisfies

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$$a(e_N, v; \mu) = r_N(v; \mu), \qquad \forall\, v \in Y,$$

and, for any $\mu \in \mathcal{D}$ and $\alpha_{\mathrm{LB}}(\mu) \le \alpha(\mu)$, we have

$$\|e_N(\mu)\|_Y \ \le \ \underbrace{\frac{\|r_N(\cdot;\mu)\|_{Y'}}{\alpha_{\mathrm{LB}}(\mu)}}_{=:\ \Delta_N^y(\mu)} \qquad \text{and} \qquad |s - s_N| \ \le \ \underbrace{\|\ell\|_{Y'} \Delta_N^y}_{=:\ \Delta_N^\ell(\mu)}$$

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How do we compute $y_N, s_N, \Delta_N^y, \Delta_N^\ell$ efficiently?

(3) Offline/Online Decomposition

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

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$$\underbrace{A_N(\mu)}_{\text{RB-MATRIX}} = Z_N^T \underbrace{A(\mu)}_{\text{FE-MATRIX}} Z_N = \sum_{q=1}^{Q} \theta^q(\mu) \underbrace{Z_N^T A^q Z_N}_{\mu\text{-INDEPENDENT}}$$

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Similarly

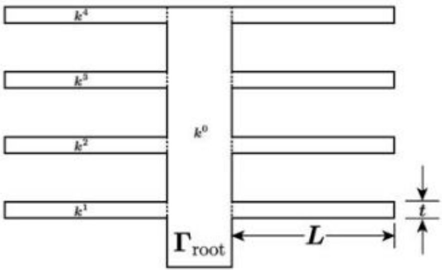
$$F_N(\mu) = Z_N^T F(\mu) = \sum_{q=1}^{Q_f} \theta_f^q(\mu)\, Z_N^T F^q$$

and

$$L_N(\mu) = Z_N^T L(\mu) = \sum_{q=1}^{Q_\ell} \theta_\ell^q(\mu)\, Z_N^T L^q$$

(3) Offline/Online Decomposition – Example

Affine Parameter Dependence: Example 1



Parameters:

$$\mu = (\underbrace{k^0, k^1, k^2, k^3, k^4}_{\text{THERMAL CONDUCTIVITIES}})$$

Governing Equation:

$$-k^i \nabla^2 y_i = 0$$

in Ω_i, $i = 0$ to 4

(3) Offline/Online Decomposition – Example

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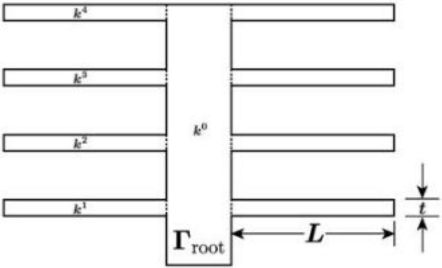

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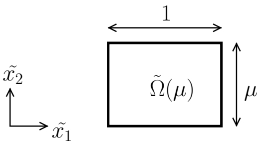
in Ω_i, $i = 0$ to 4

The matrix $A(\mu)$ then represents the bilinear form

$$a(v, w; \mu) = \sum_{i=0}^{4} \underbrace{k^i}_{\theta^q(\mu)} \underbrace{\int_{\Omega_i} \nabla v \cdot \nabla w}_{\text{“=”} A^q}$$

(3) Offline/Online Decomposition – Example

Affine Parameter Dependence: Example 2



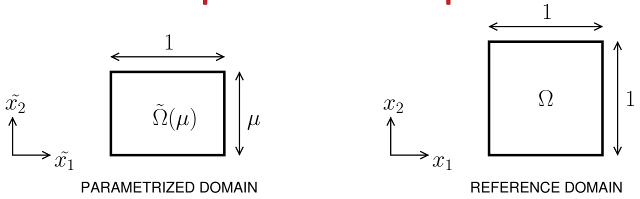
PARAMETRIZED DOMAIN

Bilinear Form on Parameter-Dependent Domain

$$\tilde{a}(\tilde{v}, \tilde{w}; \mu) = \int_{\tilde{\Omega}(\mu)} \underbrace{\left(\frac{\partial \tilde{v}}{\partial \tilde{x}_1} \frac{\partial \tilde{w}}{\partial \tilde{x}_1} + \frac{\partial \tilde{v}}{\partial \tilde{x}_2} \frac{\partial \tilde{w}}{\partial \tilde{x}_2} \right)}_{\tilde{\nabla} \tilde{v} \cdot \tilde{\nabla} \tilde{w}} \, d\tilde{\Omega}(\mu), \quad \tilde{v}, \tilde{w} \in H^1(\tilde{\Omega}(\mu))$$

(3) Offline/Online Decomposition – Example

Affine Parameter Dependence: Example 2



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After (Affine) Mapping to a Reference Domain

$$a(v,w;\mu) = \int_{\Omega} \left(\frac{\partial v}{\partial x_1}\frac{\partial w}{\partial x_1} + \frac{1}{\mu^2}\frac{\partial v}{\partial x_2}\frac{\partial w}{\partial x_2}\right) \mu d\Omega, \qquad v,w \in H^1(\Omega)$$

(3) Offline/Online Decomposition: Approximation

Summary computational cost: $(Q = Q_a + Q_f)$

Offline — once, parameter *independent*

1. solve for ζ_n $\mathcal{O}(N_{\max}\mathcal{N}^{\bullet})$
2. form and store: A_N^q, $1 \le q \le Q_a$ $\mathcal{O}(QN^2\mathcal{N})$
   (same for F_N^q and L_N^q)

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   (same for F_N^q and L_N^q)

Online — many times, parameter *dependent*

1. form RB matrices: $A_N(\mu)$, $F_N(\mu)$, $L_N(\mu)$ $\mathcal{O}(QN^2)$
2. solve for $\underline{\mathrm{y}}_N(\mu)$: $\mathbf{A}_N(\mu)\,\underline{\mathrm{y}}_N(\mu) = \mathbf{F}_N(\mu)$ $\mathcal{O}(N^3)$
3. evaluate output: $s_N(\mu) = L_N^T(\mu)\underline{\mathrm{y}}_N(\mu)$ $\mathcal{O}(N)$

Online cost is independent of $\mathcal{N}$.

(3) Offline/Online Decomposition: Error Bounds

Crucial ingredient: Dual norm of residual $\|r_N(\cdot;\mu)\|_{Y'}$

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

and obtain from the definition of the residual and affine dependence

$$
\begin{aligned}
r_N(v;\mu) &= f(v) - a(y_N(\mu), v; \mu) \\
&= f(v) - a\Big(\sum_{n=1}^{N} y_{N\,n}(\mu)\zeta_n, v; \mu\Big) \\
&= f(v) - \sum_{n=1}^{N} y_{N\,n}(\mu)\, a(\zeta_n, v; \mu) \\
&= f(v) - \sum_{n=1}^{N} y_{N\,n}(\mu) \sum_{q=1}^{Q_a} \theta_a^q(\mu)\, a^q(\zeta_n, v)
\end{aligned}
$$

For simplicity, we assume here that $f(v)$ does not depend on μ.

(3) Offline/Online Decomposition: Error Bounds

Riesz representation:

$$
\begin{aligned}
(\hat{e}(\mu), v)_Y &= r_N(v;\mu) \\
&= f(v) - \sum_{q=1}^{Q_a} \sum_{n=1}^{N} \theta_a^q(\mu) y_{N\,n}(\mu) a^q\big(\zeta_n, v\big),
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\end{aligned}
$$

Linear Superposition:

$$
\Rightarrow \quad \hat{e}(\mu) = \mathcal{C} + \sum_{q=1}^{Q_a} \sum_{n=1}^{N} \theta_a^q(\mu) y_{N\,n}(\mu) \mathcal{A}_n^q
$$

where

$$
\begin{aligned}
(\mathcal{C}, v)_Y &= f(v), && \forall v \in Y; \\
(\mathcal{A}_n^q, v)_Y &= -a^q(\zeta_n, v), && \forall v \in Y, \\
& && 1 \le n \le N, 1 \le q \le Q_a.
\end{aligned}
$$

(3) Offline/Online Decomposition: Error Bounds

Thus

$$\|\hat{e}(\mu)\|_Y^2 = \left(\mathcal{C} + \sum_{q=1}^{Q_a} \sum_{n=1}^{N} \theta_a^q(\mu) y_{N\,n}(\mu) \mathcal{A}_n^q \,, \; \cdot \; \right)_Y$$

$$=$$

(3) Offline/Online Decomposition: Error Bounds

Thus

$$\|\hat{e}(\mu)\|_Y^2 = \left(\mathcal{C} + \sum_{q=1}^{Q_a} \sum_{n=1}^{N} \theta_a^q(\mu) y_{N\,n}(\mu) \mathcal{A}_n^q \, , \, \cdot \right)_Y$$

$$= (\mathcal{C}, \mathcal{C})_Y + \sum_{q=1}^{Q_a} \sum_{n=1}^{N} \theta_a^q(\mu) y_{N\,n}(\mu) \Bigg\{$$

$$2(\mathcal{C}, \mathcal{A}_n^q)_Y + \sum_{q'=1}^{Q_a} \sum_{n'=1}^{N} \theta_a^{q'}(\mu) y_{N\,n'}(\mu) (\mathcal{A}_n^q, \mathcal{A}_{n'}^{q'})_Y \Bigg\}$$

(3) Offline/Online Decomposition: Error Bounds

Offline: *once, parameter independent*

- Compute $\mathcal{C}, \mathcal{A}_n^q,\ 1 \le n \le N_{\max},\ 1 \le q \le Q_a$, from

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\end{aligned}$$

- Form/Store $(\mathcal{C}, \mathcal{C})_Y,\ (\mathcal{C}, \mathcal{A}_n^q)_Y,\ (\mathcal{A}_n^q, \mathcal{A}_{n'}^{q'})_Y$,

$$1 \le n, n' \le N_{\max}, 1 \le q, q' \le Q_a.$$

Complexity depends on N, Q_a, and $\mathcal{N}$.

(3) Offline/Online Decomposition: Error Bounds

Online: *many times, for each new μ*

(and associated solution $y_N(\mu)$)

- Evaluate

$$\|\hat{e}(\mu)\|_Y^2 = (\mathcal{C},\mathcal{C})_Y + \sum_{q=1}^{Q_a}\sum_{n=1}^{N} \theta_a^q(\mu) y_{N\,n}(\mu) \Big\{ 2(\mathcal{C},\mathcal{A}_n^q)_Y + \sum_{q'=1}^{Q_a}\sum_{n'=1}^{N} \theta_a^{q'}(\mu) y_{N\,n'}(\mu) (\mathcal{A}_n^q,\mathcal{A}_{n'}^{q'})_Y \Big\}$$

– $\mathcal{O}(Q_a^2 N^2)$

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– $\mathcal{O}(Q_a^2 N^2)$

Complexity depends on N, Q_a, but not $\mathcal{N}$.

How do we choose the snapshots?

(4) (Weak) Greedy Algorithm

Given $\boldsymbol{Y_2} = \operatorname{\mathbf{span}}\{\boldsymbol{y}(\boldsymbol{\mu_1}), \boldsymbol{y}(\boldsymbol{\mu_2})\}$, how do we choose $\boldsymbol{\mu_3}$?

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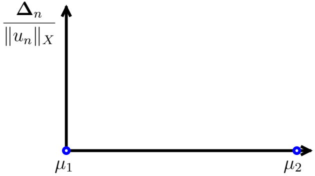

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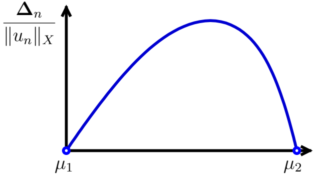

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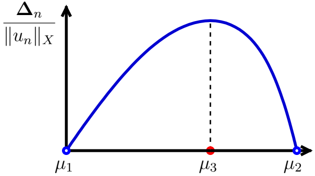

$$\boldsymbol{\mu_3} = \arg\max_{\boldsymbol{\mu} \in \boldsymbol{\mathcal{D}}_\mathbf{s}} \frac{\boldsymbol{\Delta_2}(\boldsymbol{\mu})}{\|\boldsymbol{y_2}(\boldsymbol{\mu})\|_{\boldsymbol{Y}}}$$

where $\boldsymbol{\mathcal{D}}_\mathbf{s} \subset \boldsymbol{\mathcal{D}}$ is a finite train sample

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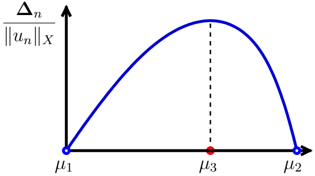
Given $Y_2 = \text{span}\{y(\mu_1), y(\mu_2)\}$, how do we choose μ_3?



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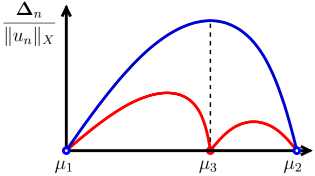

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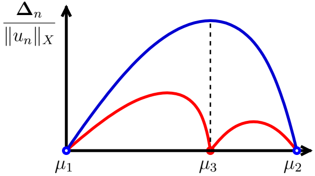

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Key points:

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

Parabolic Problems

We wish to compute, for any $\mu \in \mathcal{D}$, $t \in (0, t_f]$

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

where $y(t;\mu) \in \mathcal{Y}$, satisfies $y(0;\mu) = 0$

$$m(y_t(t;\mu), v) + a(y(t;\mu), v; \mu) = f(v)g(t), \ \forall v \in \mathcal{Y}.$$

for given $g(\cdot) \in L^2(0, t_f)$ and

$f(v), \ \ell(v)$	are bounded linear functionals
$m(\cdot,\cdot) : Y \times Y \to \mathbb{R}$	is continuous and coercive
$a(\cdot,\cdot;\mu) : Y \times Y \to \mathbb{R}$	is continuous and coercive

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

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  - FE-space Y
  - time grid $t^k = k\,\Delta t$, $0 \le k \le K$, $K = t_f/\Delta t$

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- POD/Greedy algorithm to construct $Y_N \subset Y$
- Error bound for space-time energy norm
- Online cost: $\mathcal{O}(QN^2 + N^3 + KN^2)$ plus $\mathcal{O}(KQ^2N^2)$.

Summary

The **reduced basis method** provides

accurate	$y_N \approx y$	(1) APPROX
reliable	$\Delta_N^y \geq \|y - y_N\|_Y$	(2) ERR EST
efficient surrogates	cost $O(N^*)$	(3) DECOMP
	N small	(4) GREEDY

to solutions of **parametrized PDEs**

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

and **slim-computing** contexts.

Summary

Computational Opportunities

I. We restrict our attention to the typically smooth and low-dimensional manifold induced by the parametric dependence.

$\Rightarrow$ Dimension reduction

II. We accept greatly increased offline cost in exchange for greatly decreased online cost.

$\Rightarrow$ Real-time and/or many-query context

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Note: Strict offline-online separation not always the best choice

$\Rightarrow$ adaptive or "on-the-fly" training (e.g. trust-region RB)

Part II

Data Assimilation: 4D-Var

4D-Var

Classical 4D-Var

$$\min_{u \in U} \frac{1}{2}(u - u_{\mathrm{b}})^T B^{-1}(u - u_{\mathrm{b}}) + \frac{\lambda}{2}\sum_{k=1}^{K} \Delta t (Hy^k - z_{\mathrm{d}}^k)^T D^{-1}(Hy^k - z_{\mathrm{d}}^k)$$

$$\text{s.t.} \quad y^k = \mathcal{M}(y^{k-1}), \quad k = 1, \ldots, K$$

$$y^0 = u$$

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u	initial condition
u_{b}	prior (background) estimate to the initial condition
B	covariance of the background error

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$\mathcal{M}$	model of the dynamics

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- Incorporates data in space and time (**4D**)

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- Given prior (background) estimate, data, and the model,

  find an estimate to the initial condition u^*.

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[Le Dimet 1981], [Lewis & Derber 1985], [Courtier 1985],
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[Le Dimet 1981], [Lewis & Derber 1985], [Courtier 1985], [Le Dimet & Talagrand 1986], ... [Law & Stuart 2015], [Reich 2015]

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- Assume B and D are positive-definite

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4D-Var(μ)

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$y^0 = u$

- Assume B and D are positive-definite
- Consider an FE model approximating a parabolic PDE that depends on an **unknown parameter** μ

4D-Var

4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u \in U} \frac{1}{2}\|u - u_{\mathrm{b}}\|_U^2 + \frac{\lambda}{2}\sum_{k=1}^{K} \Delta t \|H y^k - z_{\mathrm{d}}^k\|_D^2$$

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

$$y^0 = u$$

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

- Assume B and D are positive-definite
- Consider an FE model approximating a parabolic PDE that depends on an **unknown parameter** μ

4D-Var

4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u \in U} \frac{1}{2}\|u - u_{\mathrm{b}}\|_U^2 + \frac{\lambda}{2}\sum_{k=1}^{K} \Delta t \|Hy^k - z_{\mathrm{d}}^k\|_D^2$$

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

$$y^0 = u$$

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

- Assume B and D are positive-definite
- Consider an FE model approximating a parabolic PDE that depends on an **unknown parameter** μ
- Two-level optimization problem

4D-Var

4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u \in U} \frac{1}{2} \|u(\mu) - u_{\mathrm{b}}\|_U^2 + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \|H y^k(\mu) - z_{\mathrm{d}}^k\|_D^2$$

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

$$y^0 = u$$

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

4D-Var

4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u \in U} \frac{1}{2} \|u(\mu) - u_{\rm b}\|_U^2 + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \|H y^k(\mu) - z_{\rm d}^k\|_D^2$$

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

$$y^0 = u$$

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

Order Reduction for:

- PDE governing model dynamics: $Y_N \subset Y$
- Optimization space: $U_N \subset U$ ... with Greedy Algorithm

4D-Var

Reduced-Order 4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u_N \in U_N} \frac{1}{2} \| u_N(\mu) - u_\mathrm{b} \|_U^2 + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \| H y_N^k(\mu) - z_\mathrm{d}^k \|_D^2$$

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

$$\forall\, v \in Y_N,\ 1 \le k \le K$$

$$y_N^0 = u_N$$

for μ_N^* and the estimate $(u_N^*(\mu_N^*), y_N^*(\mu_N^*))$.

Order Reduction for:

- PDE governing model dynamics: $Y_N \subset Y$
- Optimization space: $U_N \subset U$ ... with Greedy Algorithm

4D-Var

Reduced-Order 4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u_N \in U_N} \frac{1}{2} \| u_N(\mu) - u_\mathrm{b} \|_U^2 + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \| H y_N^k(\mu) - z_\mathrm{d}^k \|_D^2$$

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

$$y_N^0 = u_N$$

for μ_N^* and the estimate $(u_N^*(\mu_N^*), y_N^*(\mu_N^*))$.

Order Reduction for:

- PDE governing model dynamics: $Y_N \subset Y$
- Optimization space: $U_N \subset U$ ... with Greedy Algorithm

[Robert, Durbiano, Blayo, Verron, Blum, Le Dimet 2005], [Chen, Navon, Fang 2009]
[Dimitriu, Apreutesei, Stefanescu 2010], [Stefanescu, Sandu, Navon 2015]

4D-Var

Reduced-Order 4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u_N \in U_N} \frac{1}{2} \|u_N(\mu) - u_{\rm b}\|_U^2 + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \|H y_N^k(\mu) - z_{\rm d}^k\|_D^2$$

$$\text{s.t.} \quad m(y_N^k, v) = m(y_N^{k-1}, v) - \Delta t a(y_N^k, v; \mu) + \Delta t f(v),$$
$$\forall\, v \in Y_N,\ 1 \le k \le K$$
$$y_N^0 = u_N$$

for μ_N^* and the estimate $(u_N^*(\mu_N^*), y_N^*(\mu_N^*))$.

4D-Var

Reduced-Order 4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u_N \in U_N} \frac{1}{2}\|u_N(\mu) - u_\mathrm{b}\|_U^2 + \frac{\lambda}{2}\sum_{k=1}^{K} \Delta t \|H y_N^k(\mu) - z_\mathrm{d}^k\|_D^2$$

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

$$\forall\, v \in Y_N,\ 1 \le k \le K$$

$$y_N^0 = u_N$$

for μ_N^* and the estimate $(u_N^*(\mu_N^*), y_N^*(\mu_N^*))$.

Can we quantify the error for a given μ?

CONTROL	$\|u^*(\mu) - u_N^*(\mu)\|_U$	$\le$	$\Delta_N^u(\mu)$
STATE	$\|y^*(\mu) - y_N^*(\mu)\|_Y$	$\le$	$\Delta_N^y(\mu)$

4D-Var

4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u \in U} \frac{1}{2} \|u(\mu) - u_{\mathrm{b}}\|_U^2 + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \|H y^k(\mu) - z_{\mathrm{d}}^k\|_D^2$$

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

$$\forall\, v \in Y,\ 1 \le k \le K$$

$$y^0 = u$$

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

4D-Var

4D-Var(μ)

Solve

$$\min_{\mu \in \mathcal{D}} \min_{u \in U} \frac{1}{2} \|u(\mu) - u_\mathrm{b}\|_U^2 + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \|H y^k(\mu) - z_\mathrm{d}^k\|_D^2$$

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

$$\forall\, v \in Y,\ 1 \le k \le K$$

$$y^0 = u$$

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

Lagrangian

$$\mathcal{L}(y, p, u; \mu) = \frac{1}{2} \|u - u_\mathrm{b}\|_U^2 + \frac{\lambda}{2} \sum_{k=1}^{K} \Delta t \|H y^k - z_\mathrm{d}^k\|_D^2$$

$$+ \sum_{k=1}^{K} m(y^k, p^k) - m(y^{k-1}, p^k) + \Delta t a(y^k, p^k) - \Delta t f(p^k),$$

4D-Var

Reduced Optimality Conditions

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

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

4D-Var

Reduced Optimality Conditions

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

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

We also require

- Lower bound of the a-coercivity constant

$$
\alpha_a^{\mathrm{LB}}(\mu) \le \alpha_a(\mu), \quad \forall \mu \in \mathcal{D}
$$

- Continuity constant of operator H

$$
\gamma_H = \sup_{v \in Y} \frac{\|Hv\|_D}{\|v\|_Y}
$$

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 $$e_u(\mu) := u^*(\mu) - u_N^*(\mu)$$

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 $$e_u(\mu) := u^*(\mu) - u_N^*(\mu)$$

Error-Residual Equations

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

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

CONTROL $$r_u(\psi;\mu) = (e_u, \psi)_U - m(\psi, e_p^1)$$

4D-Var

A Posteriori Error Estimation

We can show that

$$\|\boldsymbol{u}^*(\boldsymbol{\mu}) - \boldsymbol{u}^*_N(\boldsymbol{\mu})\|_U \quad \leq \quad \boldsymbol{\Delta}^u_N = \boldsymbol{c}_1(\boldsymbol{\mu}) + \sqrt{\boldsymbol{c}_1(\boldsymbol{\mu})^2 + \boldsymbol{c}_2(\boldsymbol{\mu})}$$

A Posteriori Error Estimation

We can show that

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

with non-negative terms

$$c_1 \quad := \quad \frac{1}{2}\left(\|r_u\|_{U'} + \frac{1}{\sqrt{\alpha_a^{\mathrm{LB}}}} R_p\right)$$

$$c_2 \quad := \quad \left(\frac{1+\sqrt{2}}{\alpha_a^{\mathrm{LB}}} R_y R_p + \frac{\lambda\,\gamma_H^2}{2(\alpha_a^{\mathrm{LB}})^2} R_y^2\right)$$

where $R_{y,p} = \left(\Delta t \sum_{k=1}^{K} \|r_{y,p}^k\|_{Y'}^2\right)^{\frac{1}{2}}$, and r_y^k, r_p^k, r_u

are the residuals in the state, adjoint, and control equations

4D-Var

Weak-constraint 4D-Var

[Trémolet 2006]

Solve

$$\min_{u \in U} \frac{1}{2} \|u^0 - u_{\mathrm{b}}\|_U^2 + \frac{1}{2} \sum_{k=1}^{K} \Delta t \|C y^k - z_{\mathrm{d}}^k\|_D^2 + \frac{1}{2} \sum_{k=1}^{K} \Delta t \|u^k\|_\Sigma^2$$

s.t.

$$m(y^{k+1}, v) = m(y^k, v) - \Delta t a(y^k, v; \mu) + \Delta t\, f(v) + \Delta t\, b(u^k, v), \quad \forall\, v \in Y,\ 1 \le k \le K$$

$$y^0 = u^0$$

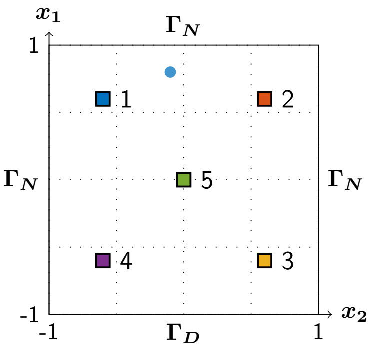
- Account for inexact model by adding a model error term, where

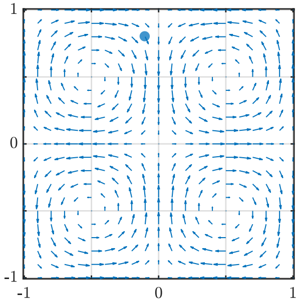
  u^k the model error in each timestep

  Σ covariance of the model error

- Allows to consider longer analysis windows

Model Problem

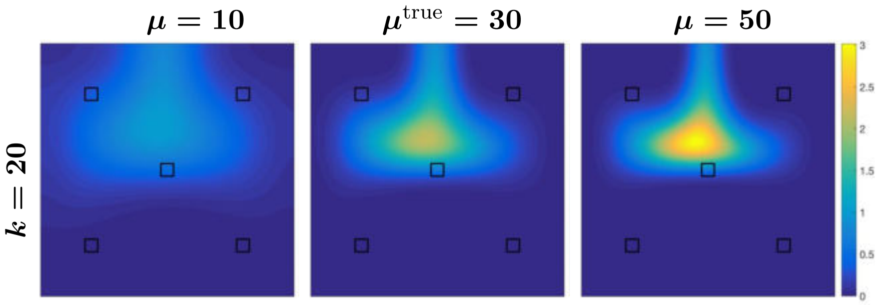




Convection-diffusion equation w. Taylor-Green vortex velocity field

Parameter	$\mu \in [10, 50]$ (Pe) with $\mu^{\text{true}} = 30$
Discretization	$\dim(Y) = \dim(U) \approx 13,000$
	time interval $I = [0, 8]$ with $\Delta t = 0.04$, $K = 400$

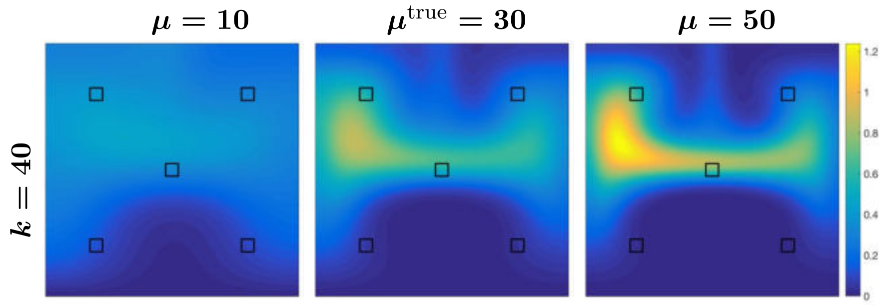
Model Problem



Assumptions

- "Gaussian" initial condition, $\bar{\boldsymbol{u}}$
- Data generated using "exact" initial condition, $\bar{\boldsymbol{u}}(\boldsymbol{\mu}^{\text{true}})$
- Prior is exact, $\boldsymbol{u}_{\text{b}} = \bar{\boldsymbol{u}}(\boldsymbol{\mu}^{\text{true}})$.
- Uncertainty due only to noise and "unknown" parameter, $\boldsymbol{\mu}^{\text{true}}$.

Model Problem



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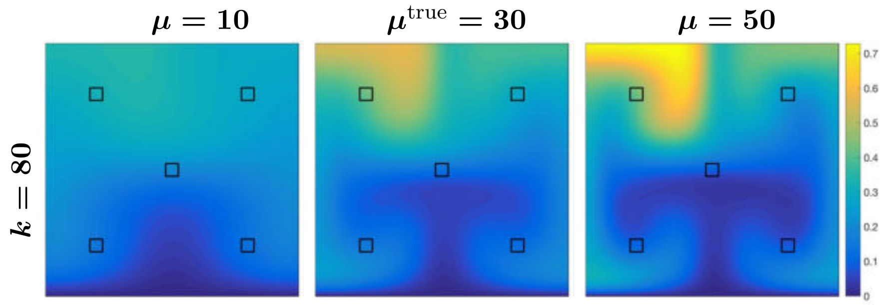
Model Problem



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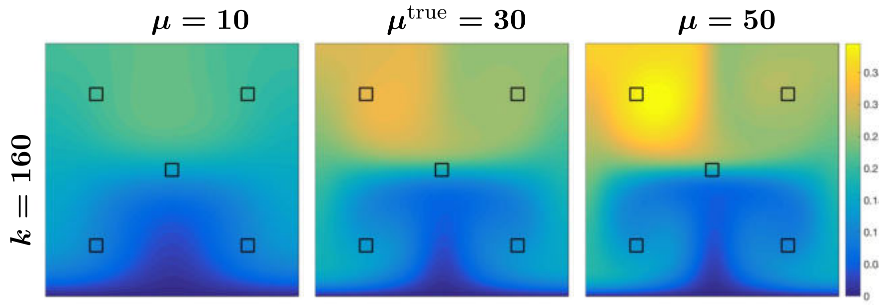
Model Problem



Assumptions

- "Gaussian" initial condition, $\bar{\boldsymbol{u}}$
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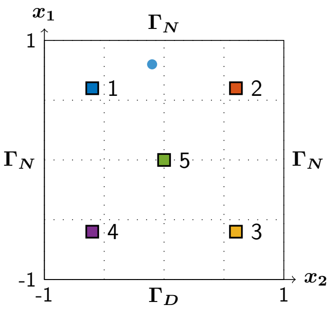
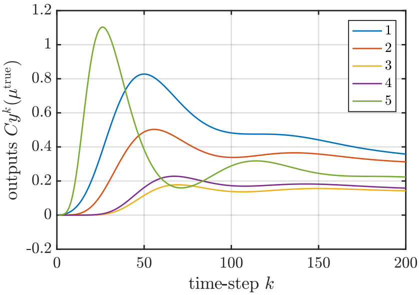
Model Problem

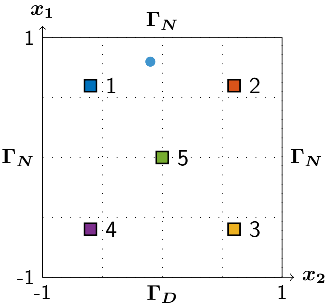


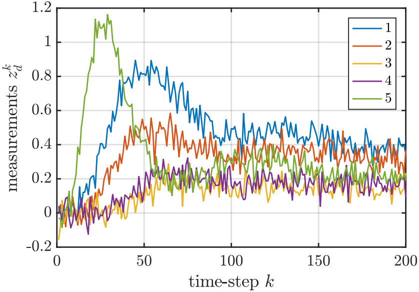


Data z_d^k $(1 \leq k \leq 800)$

- Uncorrelated Gaussian noise in each entry, $\eta \sim N(0, 0.05^2)$.

Model Problem





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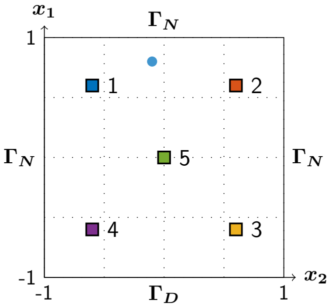
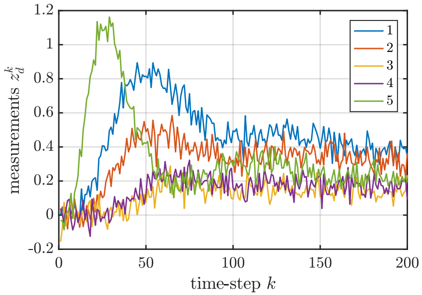
Model Problem





Data z_d^k $(1 \leq k \leq 800)$

- Uncorrelated Gaussian noise in each entry, $\eta \sim N(0, 0.05^2)$.

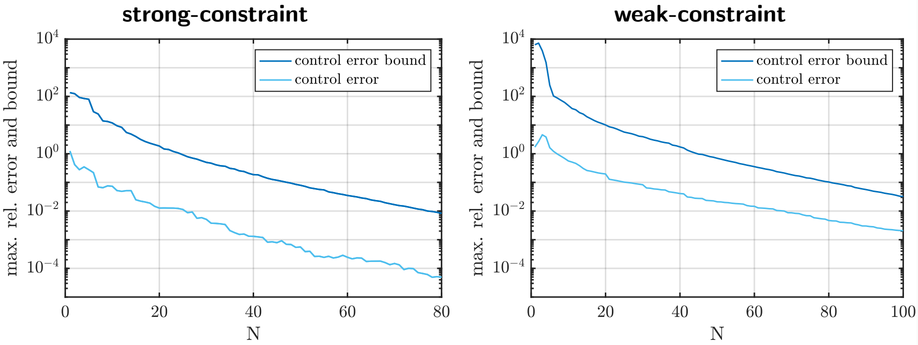
FE solution*: Preconditioned Newton-CG method

- strong-constraint: $\mathbf{30 - 54}\,\mathrm{s}$ (31 - 56 CG iterations)
- weak-constraint: $\mathbf{114 - 189}\,\mathrm{s}$ (81 - 137 CG iterations)

* Matlab, 2.6 GHz Intel Core i7 processor, 16 GB RAM

Model Problem

Convergence over test set



RB solution

- strong-constraint: $N_{Y,\max} = 2N_{\max} = 160$, $N^0_{U,\max} = 21$

  Online times: $t_{sol} \approx 10\,\text{ms} - 1.37\,\text{s}$, $t_\Delta \approx 2.8 - 29\,\text{ms}$

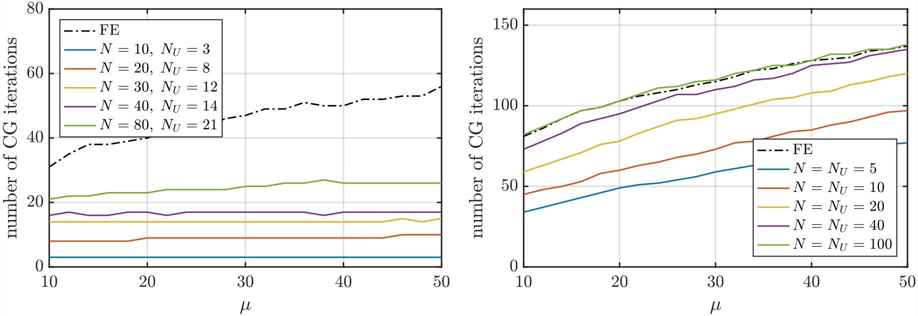
- weak-constraint: $N_{Y,\max} = 2N_{\max} = 200$, $N_{U,\max} = N_{\max} = 100$

  Online times: $t_{sol} \approx 99\,\text{ms} - 12.6\,\text{s}$, $t_\Delta \approx 4.8 - 71\,\text{ms}$

Model Problem

Required number of CG iterations

strong-constraint **weak-constraint**



Note: In the strong-constraint case

- # of CG iterations bounded by $\boldsymbol{N_U^0}$ and thus almost constant over $\boldsymbol{\mu}$
- # of RB-CG iterations $<$ # of FE-CG iterations even for $\boldsymbol{N_{\max}}$

Model Problem

Maximum relative error in cost and parameter estimate

N	$e_{J,N}^{\max}$ (strong)	$e_{\mu,N}$ (strong)	$e_{J,N}^{\max}$ (weak)	$e_{\mu,N}$ (weak)
10	3.12e-01	4.18e-01	2.44e-01	6.02e-02
20	7.36e-03	1.30e-01	1.70e-02	9.33e-03
30	8.22e-04	1.42e-03	3.51e-03	1.70e-04
40	1.24e-04	4.99e-04	6.37e-04	3.26e-04
50	1.14e-05	2.98e-05	2.05e-04	3.53e-05
60	4.36e-06	1.27e-05	9.70e-05	3.90e-05
70	3.92e-07	4.18e-06	3.58e-05	1.93e-05
80	8.76e-08	9.71e-08	1.05e-05	4.12e-06
90	-	-	4.17e-06	2.51e-06
100	-	-	1.94e-06	3.09e-06

Note:

- strong-constraint: $\mu^* = \mathbf{29.67}$
- weak-constraint: $\mu^* = \mathbf{45.36}$

Summary & Conclusions

- *A posteriori* error bounds for a reduced order approach to strong- and weak-constraint 4D-Var data assimilation
- Offline/online computational procedure for solution and bound
- Key ingredient: analogy to PDE-constrained optimal control

Summary & Conclusions

- *A posteriori* error bounds for a reduced order approach to strong- and weak-constraint 4D-Var data assimilation
- Offline/online computational procedure for solution and bound
- Key ingredient: analogy to PDE-constrained optimal control
- Cost functional & parameter estimation
  - Bound on $|\boldsymbol{J}^* - \boldsymbol{J}_N^*|$ possible based on dual-weighted residual approach
  - Bound on $|\boldsymbol{\mu}^* - \boldsymbol{\mu}_N^*|$ possible based on cost bound, but (currently) very pessimistic

Thank you for your attention!

For questions or comments:

grepl@igpm.rwth-aachen.de