

Reduced Basis Methods for Nonlinear Parametrized Partial Differential Equations

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Acknowledgments

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Outline

PART I: A Reduced Basis Primer

PART II: Nonlinear (and Nonaffine) Problems

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PART I: A Reduced Basis Primer

- ▶ Introduction
- ▶ Key Ingredients
- ▶ Extensions & References

PART II: Nonlinear (and Nonaffine) Problems

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PART I: A Reduced Basis Primer

- ▶ Introduction
- ▶ Key Ingredients
- ▶ Extensions & References

PART II: Nonlinear (and Nonaffine) Problems

- ▶ Empirical Interpolation Method
- ▶ Nonlinear Elliptic Problems
- ▶ Extensions & References
- ▶ Numerical Results
 - Nonlinear Reaction Diffusion Systems

Part I

A Reduced Basis Primer

Introduction

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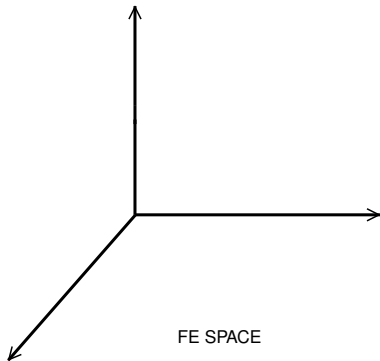
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for design and optimization, control, parameter estimation, ...

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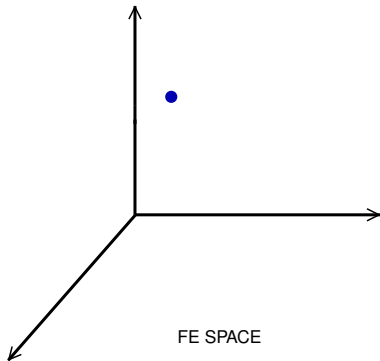
is a **model order reduction** technique that provides
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for design and optimization, control, parameter estimation, ...
— i.e., for **parameter space exploration**.

The Reduced Basis Method



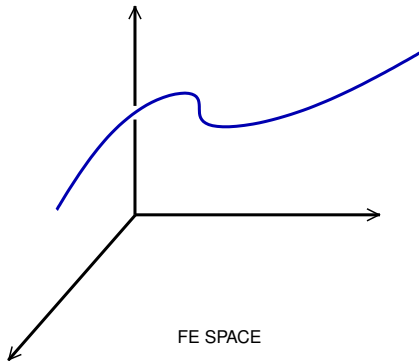
$$a(\mathbf{u}(\boldsymbol{\mu}), \mathbf{v}; \boldsymbol{\mu}) = f(\mathbf{v}; \boldsymbol{\mu}), \quad \text{for all } \mathbf{v} \in \mathcal{X}$$

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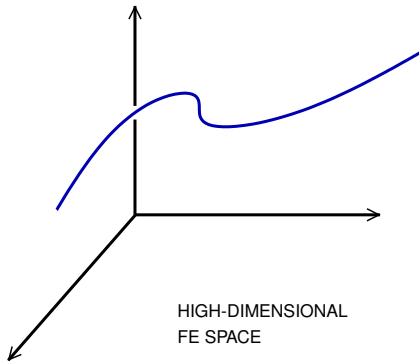
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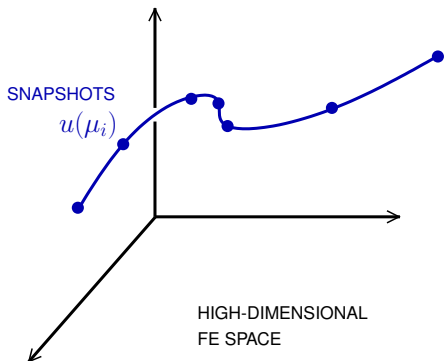
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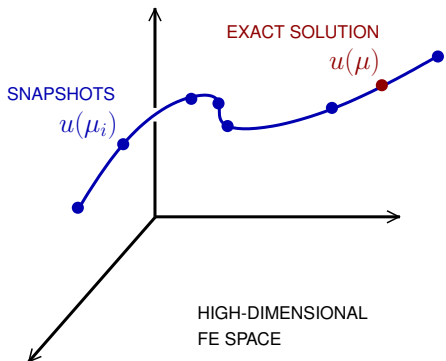
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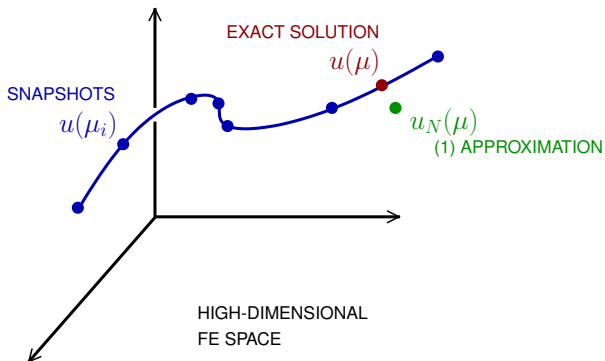
$$\mathcal{X}_N = \text{span} \{ u(\mu_i), i = 1, \dots, N \}$$

The Reduced Basis Method



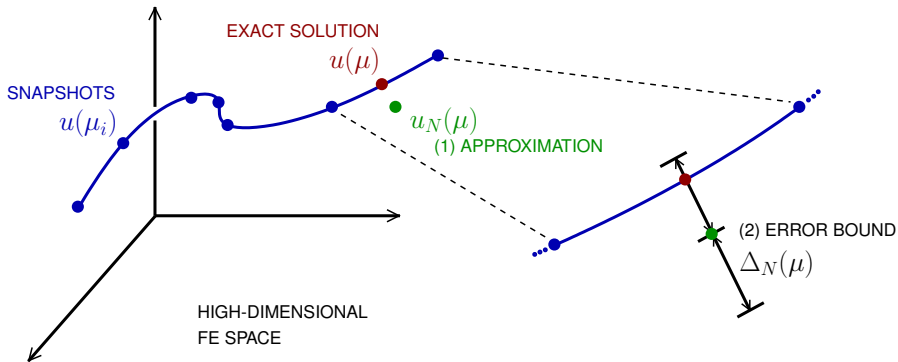
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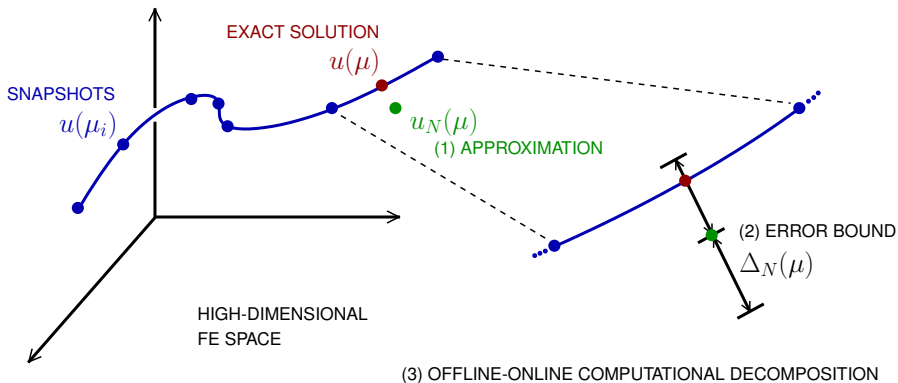
$$a(u_N(\mu), v; \mu) = f(v; \mu), \quad \text{for all } v \in \mathcal{X}_N.$$

The Reduced Basis Method



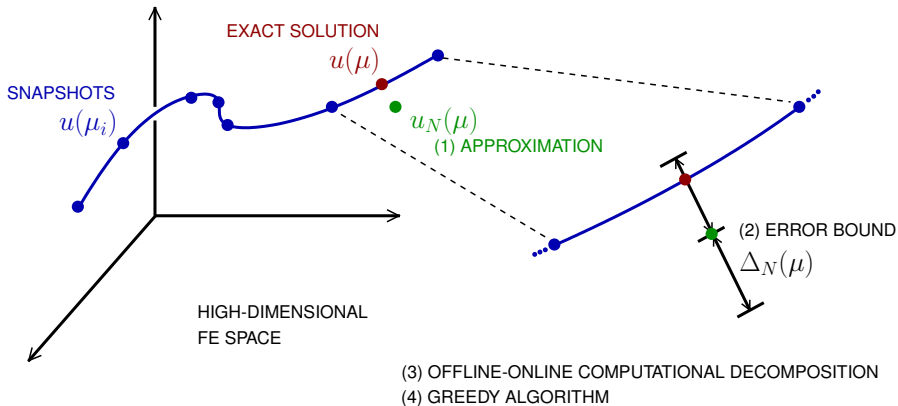
$$\|u(\mu) - u_N(\mu)\|_{\mathcal{X}} \leq \Delta_N^u(\mu) := \frac{\|r_N(\cdot; \mu)\|_{\mathcal{X}'}}{\alpha_{\text{LB}}(\mu)}$$

The Reduced Basis Method



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

The Reduced Basis Method



$$\mu_{n+1} = \arg \max_{\mu \in \mathcal{D}_s} \frac{\Delta_n^u(\mu)}{\|u_N(\mu)\|_{\mathcal{X}}}$$

Problem Statement

We wish to compute, for any parameter $\mu \in \mathcal{D}$,

$$s(\mu) = \ell(u(\mu); \mu) \quad \text{OUTPUT}$$

where $u(\mu) \in \mathcal{X}$ satisfies

$$a(u, v; \mu) = f(v; \mu), \quad \text{for all } v \in \mathcal{X}, \quad \text{FEM}_{\mathcal{N}}(\mu)$$

and

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

$a(\cdot, \cdot; \mu) : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is continuous and coercive

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

(1) Approximation

We let

$$\mathcal{X}_N = \text{span} \left\{ \underbrace{u(\mu_i)}_{\text{SNAPSHOTS}}, i = 1, \dots, N \right\}$$

SNAPSHOTS

and compute our approximation as

$$s_N(\mu) = \ell(u_N(\mu); \mu)$$

where $u_N(\mu) \in \mathcal{X}_N$ satisfies

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

(1) Approximation (Algebraic Formulation)

We let

$$\mathbf{X}_N = \left[\underbrace{\zeta_1} \quad \underbrace{\zeta_2} \quad \dots \quad \underbrace{\zeta_N} \right] \quad \text{s.t.} \quad \mathbf{u}_N(\boldsymbol{\mu}) = \mathbf{X}_N \underline{\mathbf{u}}_N(\boldsymbol{\mu})$$

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How do we quantify the error?

(2) Error Estimation

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

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

and define **residual** $r_N(v; \mu) := f(v; \mu) - a(u_N, v; \mu)$, $\forall v \in \mathcal{X}$.

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$$a(e_N, v; \mu) = r_N(v; \mu), \quad \forall v \in \mathcal{X},$$

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

$$\|e_N(\mu)\|_{\mathcal{X}} \leq \underbrace{\frac{\|r_N(\cdot; \mu)\|_{\mathcal{X}'}}{\alpha_{\text{LB}}(\mu)}}_{=: \Delta_N^u(\mu)} \quad \text{and} \quad |s - s_N| \leq \underbrace{\|\ell\|_{\mathcal{X}'} \Delta_N^u}_{=: \Delta_N^\ell(\mu)}$$

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How do we compute $u_N, s_N, \Delta_N^u, \Delta_N^\ell$ efficiently?

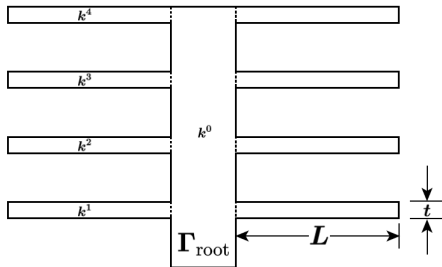
(3) Offline/Online Decomposition

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

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

(3) Offline/Online Decomposition – Example

Affine Parameter Dependence: Example 1



Parameters:

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

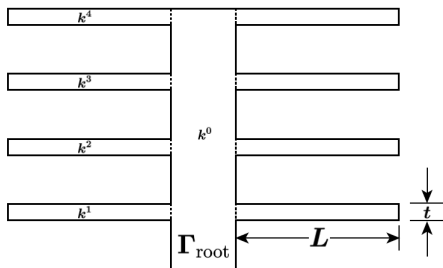
Governing Equation:

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

$$\text{in } \Omega_i, \quad i = 0 \text{ to } 4$$

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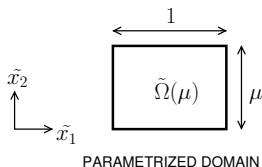
in Ω_i , $i = 0$ to 4

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

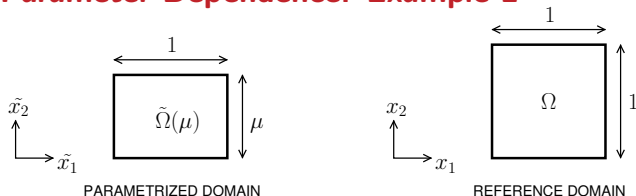


Bilinear Form on Parameter-Dependent Domain

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

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After (Affine) Mapping to a Reference Domain

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

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

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Since all required quantities can be decomposed in this manner, we can

OFFLINE: Form and store μ -independent quantities
at cost $O(\mathcal{N}^*)$

ONLINE: For any $\mu \in \mathcal{D}$, compute approx and error bounds
at cost $O(QN^2 + N^3)$ and $O(Q^2N^2)$

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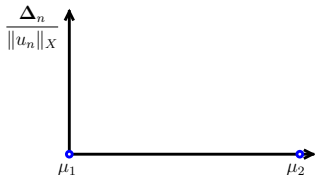
How do we choose the snapshots?

(4) (Weak) Greedy Algorithm

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

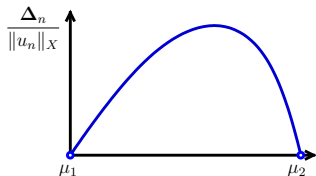
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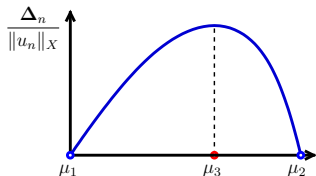
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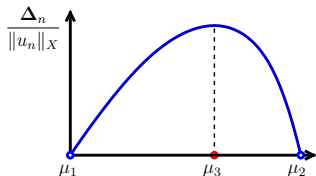


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where $\mathcal{D}_s \subset \mathcal{D}$ is a finite train sample

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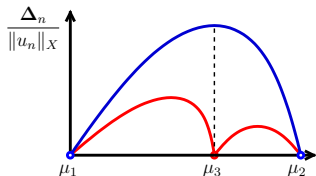
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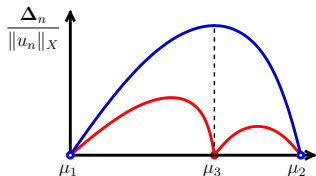
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Key points:

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

Summary

The **reduced basis method** provides

accurate

$$u_N \approx u \quad \text{APPROX}$$

reliable

$$\Delta_N \geq \|u - u_N\|_{\mathcal{X}} \quad \text{ERR EST}$$

efficient surrogates

$$\text{cost } O(N^*) \quad \text{DECOMP}$$

$$N \text{ small} \quad \text{GREEDY}$$

to solutions of **parametrized PDEs**

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

and **slim-computing** contexts.

Extensions & References

Review Articles: [RHP08], [QRM11], ...

Book: [HRS15]

Reduced Basis Methods for:

- ▶ **elliptic coercive** [PRV⁺02], [PRVP02], ...
- ▶ **elliptic noncoercive** [VPRP03], [MPR02], ...
- ▶ **saddle point (Stokes)** [Rov03], [RV07], [GV12], ...
- ▶ **parabolic** [GP05], [RMM06], [HO08], [UP14], ...
- ▶ **hyperbolic (transport-dominated)** [PR07], [HKP11], [DPW14], ...

Disclaimer:

- ▶ List contains – to the best of my knowledge – only the first papers on these topics and is thus not meant to be exhaustive
- ▶ References to nonaffine and nonlinear problems to follow ...

Extensions & References

References by topic for:

- ▶ **error bounds (adjoint techniques)** [PRV⁺02], [GP05], ...
- ▶ **stability factor lower bounds** [VRP02], [HRSP07], [HKC⁺10], [CHMR09],
- ▶ *a priori* **convergence** [MPT02], ...
- ▶ **greedy algorithm**
 - original paper [VPRP03]
 - convergence analysis [BMP⁺12], [BCD⁺11], [DPW12], [Haa13], ...
 - variations (hpRB, ...) [EPR10], [BTWGvBW07], [BTWG08], ...
- ▶ **geometry parametrization** [RHP08], [LR10], ...
- ▶ **multiscale problems** [Ngu08]
- ▶ **stochastic problems** [BBM⁺09], [BBL⁺10]
- ▶ ...

Disclaimer: see previous slide ...

Part II

Nonlinear (and Nonaffine) Problems

Nonlinear Problems

Distinguish between problems involving

- ▶ **quadratic nonlinearities**

- ▶ **higher-order or nonpolynomial nonlinearities**

Nonlinear Problems

Distinguish between problems involving

▶ quadratic nonlinearities

- (Petrov-)Galerkin projection
- *A posteriori* error bounds: Brezzi-Rappaz-Raviart [BRR80]
- Offline/online: dominant online cost $O(N^4)$
- Ref.: [VPP03], [VP05], [Dep08], [DL12], [RG12], [MPU14], [Yan14], . . .

▶ higher-order or nonpolynomial nonlinearities

Nonlinear Problems

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► quadratic nonlinearities

- (Petrov-)Galerkin projection
- *A posteriori* error bounds: Brezzi-Rappaz-Raviart [BRR80]
- Offline/online: dominant online cost $\mathcal{O}(N^4)$
- Ref.: [VPP03], [VP05], [Dep08], [DL12], [RG12], [MPU14], [Yan14], ...

► higher-order or nonpolynomial nonlinearities

- Additional approximation of nonlinearity (EIM)
- *A posteriori* error estimation (in general no bounds)
- Offline-online decomposition possible
- References: to follow ...

Problem Statement

We wish to compute, for any parameter $\mu \in \mathcal{D}$,

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

where $u(\mu) \in \mathcal{X}$ satisfies

$$a(u, v; \mu) + \int_{\Omega} g^{\text{nl}}(u; x; \mu) v = f(v), \quad \forall v \in \mathcal{X},$$

and

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

$a(\cdot, \cdot; \mu) : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is continuous and coercive

and the nonlinearity satisfies

- $g^{\text{nl}} : \mathbb{R} \times \Omega \times \mathcal{D} \rightarrow \mathbb{R}$ continuous;
- $g^{\text{nl}}(u_1; x; \mu) \leq g^{\text{nl}}(u_2; x; \mu), \forall u_1 \leq u_2;$
- $u g^{\text{nl}}(u; x; \mu) \geq 0, \forall u \in \mathbb{R},$ for any $x \in \Omega, \mu \in \mathcal{D}.$

RB-Galerkin Approximation

We let

$$\mathcal{X}_N = \text{span} \left\{ \underbrace{u(\mu_i)}_{\text{SNAPSHOTS}}, i = 1, \dots, n \right\}$$

SNAPSHOTS

and compute our approximation as

$$s_N(\mu) = \ell(u_N(\mu); \mu)$$

where $u_N(\mu) \in \mathcal{X}_N$ satisfies

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Can we still compute u_N efficiently?

RB-Galerkin Approximation

Sample Computation:

We expand $\mathbf{u}_N(\boldsymbol{\mu}) = \sum_{j=1}^N \mathbf{u}_{Nj}(\boldsymbol{\mu}) \zeta_j$,

and obtain

$$(v = \zeta_i, 1 \leq i \leq \mathcal{N})$$

$$\int_{\Omega} g^{\text{nl}}(\mathbf{u}_N(\boldsymbol{\mu}); \mathbf{x}; \boldsymbol{\mu}) \zeta_i = \int_{\Omega} g^{\text{nl}}\left(\sum_{j=1}^N \mathbf{u}_{Nj}(\boldsymbol{\mu}) \zeta_j; \mathbf{x}; \boldsymbol{\mu}\right) \zeta_i$$

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Issues

- ▶ Online assembly requires \mathcal{N} -dependent cost

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Issues

- ▶ Online assembly requires \mathcal{N} -dependent cost
- ▶ Similar to nonaffine problems: assume g^{na} is nonaffine, then

$$b(\zeta_i; \boldsymbol{\mu}) = \int_{\Omega} g^{\text{na}}(\mathbf{x}; \boldsymbol{\mu}) \zeta_i \quad \text{e.g. } e^{-\left(\frac{\mathbf{x}-\boldsymbol{\mu}}{\sigma}\right)^2}$$

requires \mathcal{N} -dependent cost.

Empirical Interpolation Method

Main Idea:

$$g^{\text{na}}(\mathbf{x}; \boldsymbol{\mu}) \approx g_M^{\text{na}}(\mathbf{x}; \boldsymbol{\mu}) = \sum_{m=1}^M \underbrace{\varphi_{M m}(\boldsymbol{\mu})}_{\text{EIM}} \underbrace{q_m(\mathbf{x})}_{\text{Collateral RB}}$$

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- ▶ How do we quantify the (interpolation) error introduced?

Empirical Interpolation Method

Greedy Procedure

[MNPP07]

Initialize: Choose $\mu_1^g \in \mathcal{D}$ and set

$$x_1^T = \arg \max_{x \in \Omega} |g(x; \mu_1^g)|, \quad q_1 = \frac{g(x; \mu_1^g)}{g(x_1^T; \mu_1^g)}.$$

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For $1 \leq M \leq M_{\max} - 1$:

► Sample Set

$$\mu_{M+1}^g \equiv \arg \max_{\mu \in \Xi_{\text{train}}^g} \|g(\cdot; \mu) - g_M(\cdot; \mu)\|_{L^\infty(\Omega)}$$

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- ▶ EIM Space

$$q_{M+1}(x) = \frac{r_{M+1}(x)}{r_{M+1}(x_{M+1}^T)}$$

Empirical Interpolation Method

Interpolation Points, Samples, and Spaces:

$$\mathbf{T}_M^g = \{x_1^T \in \Omega, \dots, x_M^T \in \Omega\},$$

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Approximation: for given $\mu \in \mathcal{D}$

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

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$$\sum_{m=1}^M q_m(x_n^T) \varphi_{M m}(\mu) = g(x_n^T; \mu), \quad 1 \leq n \leq M.$$

Note: $B_{nm}^M = q_m(x_n^T)$ lower triangular and invertible.

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How do we quantify the (interpolation) error?

Empirical Interpolation Method

“Next Point” Estimator

Given an approximation $g_M(x; \mu)$ for $M \leq M_{\max} - 1$, we define

$$\hat{\varepsilon}_M(\mu) \equiv |g(x_{M+1}^T; \mu) - g_M(x_{M+1}^T; \mu)|$$

and, if $g(\cdot; \mu) \in X_{M+1}^g$, we have

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

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- ▶ An *a posteriori* error bound exists [EGP10], but does not extend to the nonlinear case

EIM-RB-Galerkin Approximation

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

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

where $u_{N,M}(\mu) \in \mathcal{X}_N$ satisfies

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Admits **offline/online** treatment:

online cost (per Newton iteration) $\mathcal{O}(M^2 + MN^2 + N^3)$

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How do we quantify the (RB+EIM) error?

Error Estimation

Define the dual norm

$$\vartheta_M^q = \sup_{v \in \mathcal{X}} \frac{\int_{\Omega} q_{M+1} v}{\|v\|_{\mathcal{X}}}$$

and the **residual**, for all $v \in \mathcal{X}$,

$$r_{N,M}(v; \mu) := f(v) - a(u_{N,M}, v; \mu) - \int_{\Omega} g_M^{\text{nl}, u_{N,M}}(x; \mu) v.$$

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$$\|e_{N,M}(\mu)\|_{\mathcal{X}} \leq \frac{1}{\alpha_{\text{LB}}(\mu)} (\|r_{N,M}(\cdot; \mu)\|_{\mathcal{X}'} + \hat{\varepsilon}_M(\mu) \vartheta_M^q).$$

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- ▶ In general $g^{\text{nl}}(u_{N,M}; x; \mu) \notin X_{M+1}^g$, and hence the bound is more like an estimator

Nonlinear Parabolic Problems

We wish to compute, for any $\mu \in \mathcal{D}$,

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

where $u(t; \mu) \in \mathcal{Y}$, satisfies

$$u(0; \mu) = 0$$

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Key Ingredients:

- ▶ FE[x]-FD[t] truth approximation
- ▶ POD/Greedy algorithm to construct \mathcal{X}_N and X_M^g
- ▶ Error bound/estimator for space-time energy norm
- ▶ Online cost: $\mathcal{O}(M^2 + MN^2 + N^3)^\dagger$ plus $\mathcal{O}(KM^2N^2)$.

[†] Cost per Newton iteration per timestep.

Extensions & References

Empirical Interpolation Method:

- ▶ **methodology** [BMNP04], [GMNP07], [MNPP07], ...
- ▶ **error bounds** [EGP10], [EGPR13], ...
- ▶ **generalized EIM** [MM13], [MMPY15], ...
- ▶ **variations** [CS10], ...

Related Methods:

- ▶ **best points interpolation** [NPP08], ...
- ▶ **adaptive cross approximation** [Beb00], [Beb11], ...
- ▶ **gappy POD** [ES95], [BTDW04], [Wil06], [GFWG10], ...
- ▶ **missing point estimation** [AWWB08], ...

For a comparison of these methods: [BMS14]

Extensions & References

RB for nonaffine problems:

- ▶ **elliptic** [BMNP04], [GMNP07], [Ngu07], [Roz09], ...
- ▶ **parabolic** [GMNP07], [Gre12a], [KGV12], ...

RB for nonlinear problems:

- ▶ **elliptic** [GMNP07], [NP08], [CTU09], ...
- ▶ **parabolic** [GMNP07], [Gre12a], [DHO12], [Gre12b], ...

Issues

- ▶ Convergence and stability of EIM-RB approximation
- ▶ Greedy EIM algorithm requires (truth) solution at all $\mu \in \mathcal{D}_s$
- ▶ Simultaneous EIM + RB [DP15]

Model Problem

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

$$s^k(\mu) = \int_{\Omega} u^k(\mu)$$

where $u^k(\mu) \in \mathcal{X}$, $1 \leq k \leq K$, satisfies $u^0(\mu) = 0$

$$\frac{1}{\Delta t} m(u^k(\mu) - u^{k-1}(\mu), v) + a(u^k(\mu), v) + \int_{\Omega} g^{\text{nl}}(u^k(\mu); x; \mu) v = b(v) \sin(2\pi t^k), \quad \forall v \in \mathcal{X},$$

$$\text{with } g^{\text{nl}}(u^k(\mu); x; \mu) = \mu_1 \frac{e^{\mu_2 u^k(\mu)} - 1}{\mu_2}.$$

Truth Approximation:

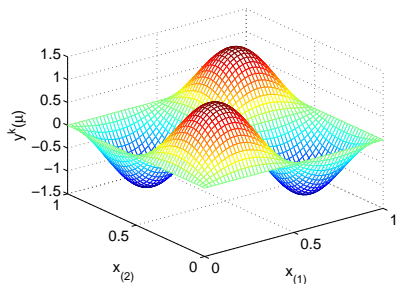
- ▶ Space: $\mathcal{X} \subset \mathcal{X}^e \equiv H_0^1(\Omega)$ with dimension $\mathcal{N} = 2601$;
- ▶ Time: $\bar{I} = (0, 2]$, $\Delta t = 0.01$, and thus $K = 200$.

Sample Results

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

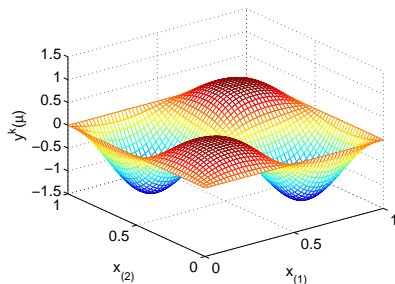
$$\mu = (0.01, 0.01)$$

Solution for $\mu = (0.01, 0.01)$, $t^k = 25 \Delta t$



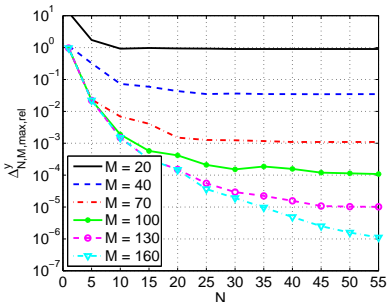
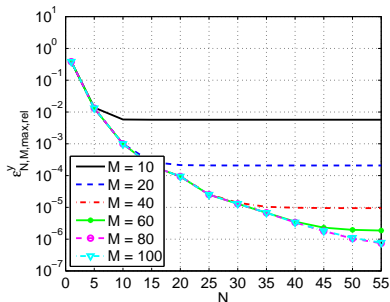
$$\mu = (10, 10)$$

Solution for $\mu = (10, 10)$, $t^k = 25 \Delta t$



$$b(v) = 100 \int_{\Omega} v \sin(2\pi x_1) \sin(2\pi x_2)$$

Convergence: Energy Norm



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

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

Convergence: Energy Norm & Output

N	M	$\epsilon_{N,M,\max,\text{rel}}^y$	$\Delta_{N,M,\max,\text{rel}}^y$	$\bar{\eta}_{N,M}^y$
1	40	3.83 E-01	1.15 E+00	2.44
5	60	1.32 E-02	4.59 E-02	2.43
10	80	9.90 E-04	3.41 E-03	2.10
20	100	9.40 E-05	4.16 E-04	2.77
40	140	3.36 E-06	8.75 E-06	1.64

N	M	$\epsilon_{N,M,\max,\text{rel}}^s$	$\Delta_{N,M,\max,\text{rel}}^s$	$\bar{\eta}_{N,M}^s$
1	40	9.99 E-01	2.49 E+01	14.1
5	60	5.35 E-03	1.00 E+00	130
10	80	2.57 E-04	7.42 E-02	146
20	100	1.43 E-05	9.06 E-03	436
40	140	2.85 E-06	1.90 E-04	205

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

Online Computational Times

N	M	$s_{N,M}(\mu, t^k)$	$\Delta_{N,M}^s(\mu, t^k)$	$s(\mu, t^k)$
1	40	5.42 E-05	9.29 E-05	1
5	60	9.67 E-05	8.58 E-05	1
10	80	1.19 E-04	9.37 E-05	1
20	100	1.71 E-04	1.05 E-04	1
40	140	3.15 E-04	1.35 E-04	1

Average CPU times for sample $\Xi_{\text{test}} \in \mathcal{D}$ of size 225.

- ▶ Computational savings $\mathcal{O}(10^3)$ for $\Delta_{N,M,\text{max,rel}}^s < 1\%$.
- ▶ **But** offline stage much more expensive than for linear case.

Nonlinear Reaction-Diffusion Systems

General formulation:

[Gre12b]

$$\frac{\partial y(x, t; \mu)}{\partial t} = \nabla(D(\mu)\nabla y(x, t; \mu)) + f(y(x, t; \mu); \mu)$$

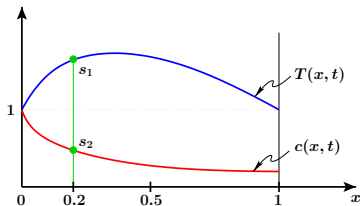
Self-ignition of a coal stockpile

$$\frac{\partial T(x, t)}{\partial t} = \nabla^2 T(x, t) + \beta \Phi^2 (c(x, t) + 1) e^{-\gamma/(T(x, t)+1)},$$

$$\frac{\partial c(x, t)}{\partial t} = \text{Le} \nabla^2 c(x, t) - \Phi^2 (c(x, t) + 1) e^{-\gamma/(T(x, t)+1)},$$

where

- γ : Arrhenius number,
- β : Prater temperature,
- Le : Lewis number,
- Φ : Thiele modulus.



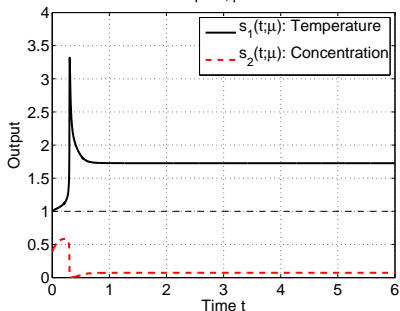
► Nonlinearity not monotonic: *a posteriori* error bounds not valid.

Nonlinear Reaction-Diffusion Systems

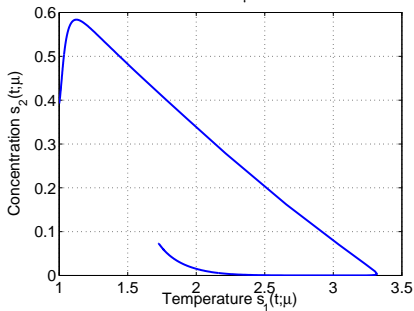
- ▶ Very complex dynamic behavior (depending on parameters).
- ▶ Here: $\mu \equiv \gamma \in [12, 12.6]$, all other parameters fixed, $\mathcal{N} = 501$

Temperature and Concentration: $\gamma = 12.0$

Outputs, $\mu = 12$



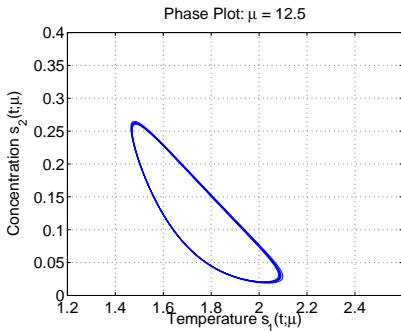
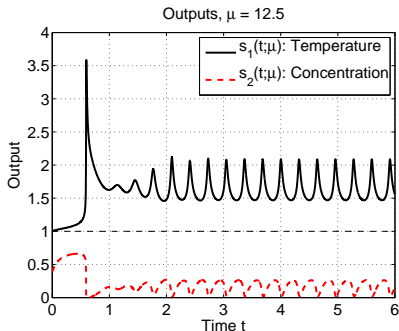
Phase Plot: $\mu = 12.0$



Nonlinear Reaction-Diffusion Systems

- ▶ Very complex dynamic behavior (depending on parameters).
- ▶ Here: $\mu \equiv \gamma \in [12, 12.6]$, all other parameters fixed, $\mathcal{N} = 501$

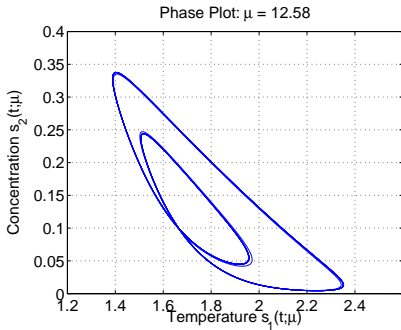
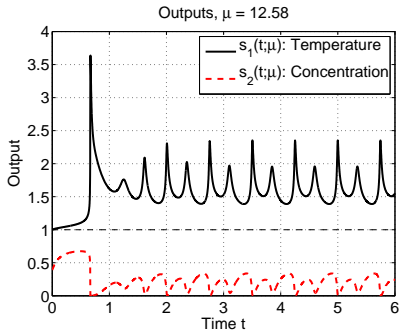
Temperature and Concentration: $\gamma = 12.5$



Nonlinear Reaction-Diffusion Systems

- ▶ Very complex dynamic behavior (depending on parameters).
- ▶ Here: $\mu \equiv \gamma \in [12, 12.6]$, all other parameters fixed, $\mathcal{N} = 501$

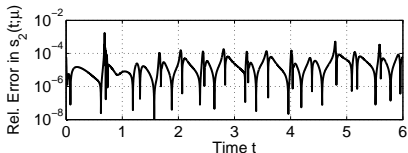
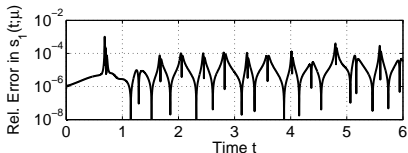
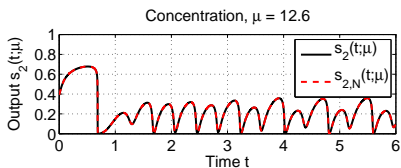
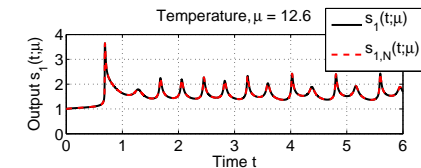
Temperature and Concentration: $\gamma = 12.58$



Nonlinear Reaction-Diffusion Systems

- ▶ Very complex dynamic behavior (depending on parameters).
- ▶ Here: $\mu \equiv \gamma \in [12, 12.6]$, all other parameters fixed, $\mathcal{N} = 501$
 $N_T = N_c = 16$, $M = 36$: $t_{RB}/t_{FEM} = 5.12 \text{E-}03$

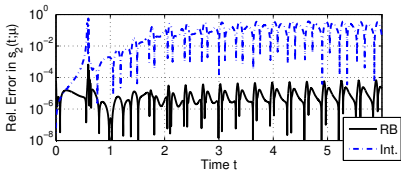
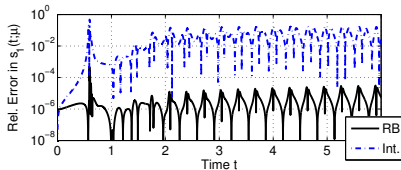
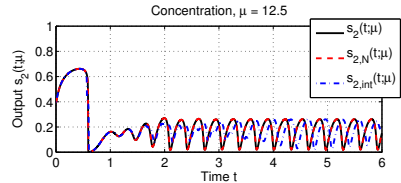
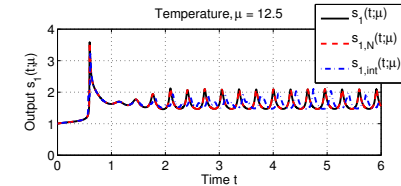
FEM solution and RB approximation: $\gamma = 12.6$



Nonlinear Reaction-Diffusion Systems

- ▶ Very complex dynamic behavior (depending on parameters).
- ▶ Here: $\mu \equiv \gamma \in [12, 12.6]$, all other parameters fixed, $\mathcal{N} = 501$
 $N_T = N_c = 16$, $M = 36$: $t_{\text{RB}}/t_{\text{FEM}} = 5.12 \text{E-}03$

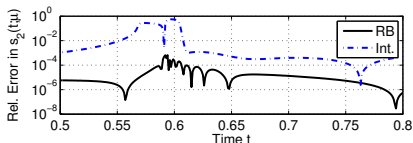
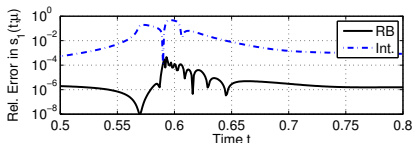
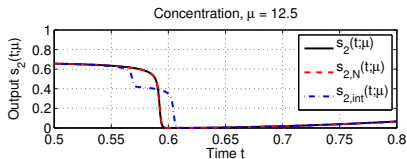
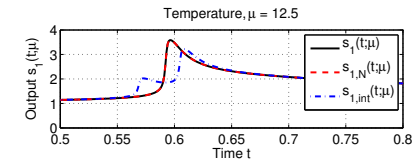
FEM, RB, and output interpolation: $\gamma = 12.5$



Nonlinear Reaction-Diffusion Systems

- ▶ Very complex dynamic behavior (depending on parameters).
- ▶ Here: $\mu \equiv \gamma \in [12, 12.6]$, all other parameters fixed, $\mathcal{N} = 501$
 $N_T = N_c = 16$, $M = 36$: $t_{RB}/t_{FEM} = 5.12 \text{E-}03$

FEM, RB, and output interpolation: $\gamma = 12.5$



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Thank you for your attention!

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Part III

Extra Slides

Offline/Online Decomposition: Error Bounds

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

We expand $u_N(\mu) = \sum_{j=1}^N u_{Nj}(\mu) \zeta_j$

and obtain from the definition of the residual and affine dependence

$$\begin{aligned}r_N(v; \mu) &= f(v) - a(u_N(\mu), v; \mu) \\ &= f(v) - a\left(\sum_{n=1}^N u_{Nn}(\mu) \zeta_n, v; \mu\right) \\ &= f(v) - \sum_{n=1}^N u_{Nn}(\mu) a(\zeta_n, v; \mu) \\ &= f(v) - \sum_{n=1}^N u_{Nn}(\mu) \sum_{q=1}^{Q_a} \theta_a^q(\mu) a^q(\zeta_n, v)\end{aligned}$$

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

Offline/Online Decomposition: Error Bounds

Riesz representation:

$$\begin{aligned}(\hat{e}(\mu), v)_{\mathcal{X}} &= r_N(v; \mu) \\ &= f(v) - \sum_{q=1}^{Q_a} \sum_{n=1}^N \theta_a^q(\mu) u_{Nn}(\mu) a^q(\zeta_n, v),\end{aligned}$$

Offline/Online Decomposition: Error Bounds

Riesz representation:

$$\begin{aligned}(\hat{e}(\mu), v)_{\mathcal{X}} &= r_N(v; \mu) \\ &= f(v) - \sum_{q=1}^{Q_a} \sum_{n=1}^N \theta_a^q(\mu) u_{Nn}(\mu) a^q(\zeta_n, v),\end{aligned}$$

Linear Superposition:

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

where

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

Offline/Online Decomposition: Error Bounds

Thus

$$\|\hat{e}(\mu)\|_{\mathcal{X}}^2 = \left(\mathbf{c} + \sum_{q=1}^{Q_a} \sum_{n=1}^N \theta_a^q(\mu) u_{Nn}(\mu) \mathcal{A}_n^q, \cdot \right)_{\mathcal{X}}$$
$$=$$

Offline/Online Decomposition: Error Bounds

Thus

$$\begin{aligned}\|\hat{e}(\mu)\|_{\mathcal{X}}^2 &= \left(\mathcal{C} + \sum_{q=1}^{Q_a} \sum_{n=1}^N \theta_a^q(\mu) u_{Nn}(\mu) \mathcal{A}_n^q, \cdot \right)_{\mathcal{X}} \\ &= (\mathcal{C}, \mathcal{C})_{\mathcal{X}} + \sum_{q=1}^{Q_a} \sum_{n=1}^N \theta_a^q(\mu) u_{Nn}(\mu) \left\{ \right. \\ &\quad \left. 2(\mathcal{C}, \mathcal{A}_n^q)_{\mathcal{X}} + \sum_{q'=1}^{Q_a} \sum_{n'=1}^N \theta_a^{q'}(\mu) u_{Nn'}(\mu) (\mathcal{A}_n^q, \mathcal{A}_{n'}^{q'})_{\mathcal{X}} \right\}\end{aligned}$$

Offline/Online Decomposition: Error Bounds

Offline: *once, parameter independent*

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

$$(\mathcal{C}, v)_{\mathcal{X}} = f(v), \quad \forall v \in \mathcal{X};$$

$$(\mathcal{A}_n^q, v)_{\mathcal{X}} = -a^q(\zeta_n, v), \quad \forall v \in \mathcal{X},$$

$$1 \leq n \leq N, 1 \leq q \leq Q_a.$$

Offline/Online Decomposition: Error Bounds

Offline: *once, parameter independent*

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

$$(\mathcal{C}, v)_{\mathcal{X}} = f(v), \quad \forall v \in \mathcal{X};$$

$$(\mathcal{A}_n^q, v)_{\mathcal{X}} = -a^q(\zeta_n, v), \quad \forall v \in \mathcal{X},$$

$$1 \leq n \leq N, 1 \leq q \leq Q_a.$$

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

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

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

Offline/Online Decomposition: Error Bounds

Online: many times, for each new μ

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

► Evaluate

$$\|\hat{e}(\mu)\|_{\mathcal{X}}^2 = (\mathcal{C}, \mathcal{C})x + \sum_{q=1}^{Q_a} \sum_{n=1}^N \theta_a^q(\mu) u_{Nn}(\mu) \left\{ \right. \\ \left. 2(\mathcal{C}, \mathcal{A}_n^q)x + \sum_{q'=1}^{Q_a} \sum_{n'=1}^N \theta_a^{q'}(\mu) u_{Nn'}(\mu) (\mathcal{A}_n^q, \mathcal{A}_{n'}^{q'})x \right\} \\ - O(Q_a^2 N^2)$$

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

Offline/Online Decomposition: Error Bounds

Summary of computational cost:

OFFLINE —

$$\begin{array}{ccc} O(Q_a N_{\max} \mathcal{N}^\bullet) & + & O(Q_a^2 N_{\max}^2 \mathcal{N}) \\ \text{solve Poisson problems} & & \text{form } \mu\text{-independent inner products} \end{array} ;$$

ONLINE —

$$\begin{array}{ccc} O(Q_a^2 N^2) & & \\ \text{evaluate } \|\hat{e}(\mu)\|_{\mathcal{X}\text{-sum}} & & ; \end{array}$$

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