

Reduced basis methods and a posteriori error estimation for parametrized PDEs: Fundamentals INTRODUCTION/OVERVIEW

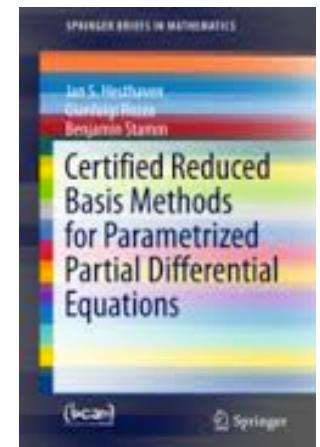
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Advanced Topics in Numerical Solution
of PDEs: Reduced Basis Methods for Computational Mechanics



References

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Outline

- ▶ **Fundamentals: Motivation, Coercive Elliptic Problems**
 - 1. Introduction/Motivation
 - (a) Notation and Examples
 - (b) Goal/Relevance
 - 2. Elliptic Problems I (coercive, affine, compliant)
 - (a) Problem Statement, Truth Approximation, Affine Representation
 - (b) Reduced Basis Approximation
 - (c) Offline-Online Computational Procedures
 - (d) Sampling/Spaces Strategies: POD, Greedy, ...

Outline

► Advances: Elliptic Problems II, Parabolic Problems

1. Elliptic Problems II

- (e) A Posteriori Error Estimation (elements)
- (f) General Outputs (non-compliant), Non-symmetric Forms
(Dual Problem, A Posteriori Error Estimation)

2. Parabolic Problems

- (a) Problem Statement, Truth Approximation
- (b) Reduced Basis Approximation
- (c) Offline-Online Computational Procedures
- (d) A Posteriori Error Estimation
- (e) POD - greedy sampling

3. Possible extensions

- (a) Stability factors estimation
- (b) Non-coercive problems

Fundamentals

► Fundamentals: Motivation, Coercive Elliptic Problems

1. Introduction/Motivation
 - (a) Notation and Examples
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2. Elliptic Problems I (coercive, affine, compliant)
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Statement: simple elliptic μ PDEs

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, evaluate $s^e(\mu) = \ell(u^e(\mu))^\dagger$

where $u^e(\mu) \in X^e$ satisfies

$$a(u^e(\mu), v; \mu) = f(v), \quad \forall v \in X^e.$$

μ : input parameter; P -tuple

\mathcal{D} : input domain;

s^e : output;

ℓ : linear bounded output functional;

u^e : field variable;

X^e : function space $(H_0^1(\Omega))^\nu \subset X^e \subset (H^1(\Omega))^\nu$;

[†]Here e refers to “exact.”

Statement: hypotheses and definitions

$a(\cdot, \cdot; \mu)$: bilinear,
continuous,
symmetric,
coercive form, $\forall \mu \in \mathcal{D}$;
 f : linear bounded functional.

$\left. \begin{array}{l} \text{bilinear,} \\ \text{continuous,} \\ \text{symmetric,} \\ \text{coercive form, } \forall \mu \in \mathcal{D}; \\ \text{linear bounded functional.} \end{array} \right\} \mu\text{PDE}$

Compliant case: $l = f$,
 $a(\cdot, \cdot; \mu)$ symmetric

Statement: hypotheses and definitions

- ▶ a symmetric: $a(u, v; \mu) = a(v, u; \mu)$,
- ▶ a bilinear: $a(\lambda u + \gamma v, w; \mu) = \lambda a(u, w; \mu) + \gamma a(v, w; \mu)$, $\forall \lambda, \gamma \in \mathbb{R}$, $\forall u, v, w \in X^e$,
or $a(u, \lambda v + \gamma w; \mu) = \lambda a(u, v; \mu) + \gamma a(u, w; \mu)$, $\forall \lambda, \gamma \in \mathbb{R}$, $\forall u, v, w \in X^e$,
- ▶ a continuous:
 $|a(u, v; \mu)| \leq M \|u\|_{X^e} \|v\|_{X^e}$, $\forall u, v \in X^e$,
- ▶ a coercive: $\exists \alpha > 0 : a(u, u; \mu) \geq \alpha^e \|u\|_{X^e}^2$, $\forall u \in X^e$,
- ▶ f (and l) bounded/continuous:
 $|f(v)| \leq C \|v\|_{X^e}$, $\forall v \in X^e$,
- ▶ f linear:
 $f(\gamma v + \eta w) = \gamma f(v) + \eta f(w)$, $\forall \gamma, \eta \in \mathbb{R}, v \in X^e$.

Statement: affine parameter dependence \dagger

Definition:

$$a(w, v; \mu) = \sum_{q=1}^Q \Theta^q(\mu) a^q(w, v)$$

for $q = 1, \dots, Q$

μ -dependent functions $\Theta^q: \mathcal{D} \rightarrow \mathbb{R}$,

μ -independent forms $a^q: X^e \times X^e \rightarrow \mathbb{R}$.

Stiffness matrix:

$$a(\begin{matrix} w \\ \zeta_j \end{matrix}, \begin{matrix} v \\ \zeta_i \end{matrix}; \mu) = \sum_{q=1}^Q \Theta^q(\mu) a^q(\begin{matrix} w \\ \zeta_j \end{matrix}, \begin{matrix} v \\ \zeta_i \end{matrix})$$

for $q = 1, \dots, Q$

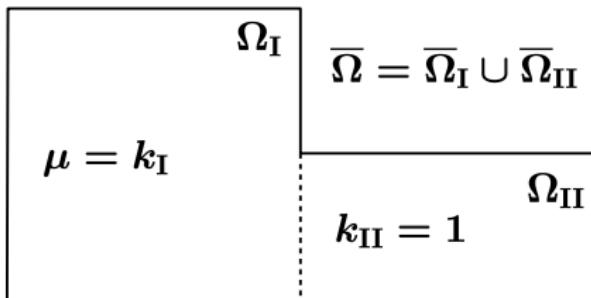
\dagger In fact, broadly applicable to many instances of geometry
and property parametric variation.

Little example: heat conduction

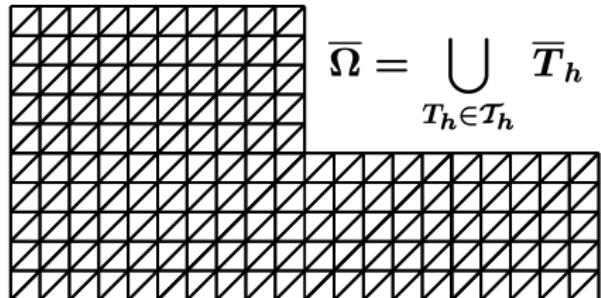
Given $k_I \in [0.1, 10]$, evaluate $\bar{u}_I^e(k_I) = \frac{1}{|\Omega_I|} \int_{\Omega_I} u^e$

where $u^e(k_I) \in H_0^1(\Omega)$ satisfies ($Q = 2$)

$$k_I \int_{\Omega_I} \nabla u^e \cdot \nabla v + \int_{\Omega_{II}} \nabla u^e \cdot \nabla v = \int_{\Omega} v, \quad \forall v \in H_0^1(\Omega).$$



$$\bar{\Omega} = \bar{\Omega}_I \cup \bar{\Omega}_{II}$$



$$X^{\mathcal{N}} \equiv \{v|_{T_h} \in \mathbb{P}_I(T_h), \forall T_h \in \mathcal{T}_h\} \cap X^e; \dim(X^{\mathcal{N}}) \equiv \mathcal{N}.$$

Classical Approximation: FEM (Galerkin projection)

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

evaluate $s^{\mathcal{N}} = \ell(u^{\mathcal{N}}(\mu))$,

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

$$a(u^{\mathcal{N}}(\mu), v; \mu) = f(v), \quad \forall v \in X^{\mathcal{N}}.$$

Typically: $|s^e(\mu) - s^{\mathcal{N}}(\mu)|$ small $\Rightarrow \mathcal{N}$ large.

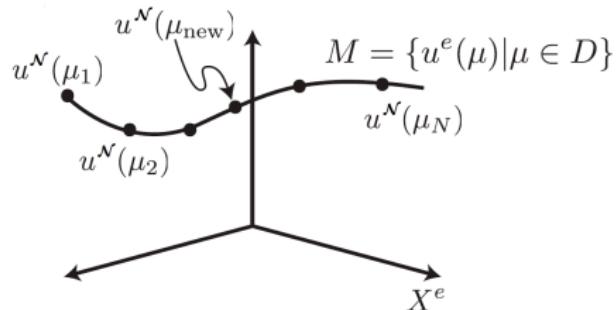
Surrogate for $s^e(\mu)$, $u^e(\mu)$:

“truth”

- ▶ upon which we *build* reduced-basis *approximation*; †
- ▶ relative to which we *measure* reduced-basis *error*. †

† Require *stability* and *efficiency* as $\mathcal{N} \rightarrow \infty$.

Reduced-Basis Approximation: basic idea †



\mathcal{M}^e = parameter-induced manifold
(low-Dimensional ($\mathcal{D} \subset \mathbb{R}^P$), very smooth)

Classical Approach

$$X^{\mathcal{N}} \equiv \{v|_{T_h} \in \mathbf{IP_I}(T_h), \forall T_h \in \mathcal{T}_h\} \cap X^e; \dim(X^{\mathcal{N}}) \equiv \mathcal{N}.$$

Reduced Basis Approach

$$W_N \equiv \text{span}\{\zeta_n \equiv u^N(\mu_n), 1 \leq n \leq N\}$$

† Pioneering works by Almroth, Stern & Brogan (1978), Noor & Peters (1980)

Reduced-Basis Approximation: formulation

Samples: $S_N = \{\mu_1 \in \mathcal{D}, \dots, \mu_N \in \mathcal{D}\}$

Spaces: $W_N = \text{span}\{\zeta_n \equiv u^N(\mu_n), 1 \leq n \leq N\}$

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

evaluate $s_N(\mu) = \ell(u_N(\mu))$,

where $u_N(\mu) \in W_N$ satisfies

$a(u_N(\mu), v; \mu) = f(v), \forall v \in W_N$.

Reduced-Basis Approximation: convergence

Classical arguments yield

$$\begin{aligned} a(u^N(\mu) - u_N(\mu), u^N(\mu) - u_N(\mu); \mu) = \\ \inf_{w_N \in W_N} a(u^N(\mu) - w_N, u^N(\mu) - w_N; \mu) \end{aligned}$$

Properties of \mathcal{M}^e suggest

$$\inf_{w_N \in W_N} a(u^N(\mu) - w_N, u^N(\mu) - w_N; \mu) \rightarrow 0$$

rapidly (exponentially): N small.

Reduced-Basis Approximation: discrete equations

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

evaluate $s_N(\mu) = \ell(u_N(\mu))$,

where $u_N(\mu) \in W_N$ satisfies

$$a(u_N(\mu), v; \mu) = f(v), \quad \forall v \in W_N.$$

Express

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

then

$$s_N(\mu) \equiv \ell(u_N(\mu)) = \sum_{j=1}^N u_{Nj}(\mu) \ell(\zeta_j)$$

where

$$\sum_{j=1}^N a(\zeta_j, \zeta_i; \mu) u_{Nj} = f(\zeta_i), \quad 1 \leq i \leq N.$$

RB Approximation: Offline-Online Procedure

Evaluation of $s_N(\mu)$ — GIVEN $\mathbf{u}_N j$, $1 \leq j \leq N$

OFFLINE: Compute ζ_j , $1 \leq j \leq N$; $O(N)$
Form/Store $\ell(\zeta_j)$, $1 \leq j \leq N$.

ONLINE: Perform sum

$$s_N(\mu) = \sum_{j=1}^N \mathbf{u}_N j(\mu) \ell(\zeta_j) \quad O(N)$$

RB Approximation: Offline-Online Procedure

Evaluation of $u_{N,j}(\mu)$, $1 \leq j \leq N$

IF $a(w, v; \mu)$ is affine,

$$\sum_{j=1}^N a(\zeta_j, \zeta_i; \mu) u_{N,j} = f(\zeta_i), \quad 1 \leq i \leq N .$$



$$\sum_{j=1}^N \left(\sum_{q=1}^Q \Theta^q(\mu) a^q(\zeta_j, \zeta_i) \right) u_{N,j} = f(\zeta_i), \quad 1 \leq i \leq N .$$

RB Approximation: Offline-Online Procedure

Evaluation of $u_{Nj}(\mu)$, $1 \leq j \leq N$

OFFLINE: Form/Store $a^q(\zeta_j, \zeta_i)$, $1 \leq i, j \leq N$,
 $1 \leq q \leq Q$. $O(N)$

ONLINE: Form $\sum_{q=1}^Q \Theta^q(\mu) a^q(\zeta_j, \zeta_i)$, $1 \leq i, j \leq N$
— $O(QN^2)$;

Solve for $u_{Nj}(\mu)$, $1 \leq j \leq N$ — $O(N^3)$.

RB Approximation: Offline-Online Procedure

... Evaluation of $u_{N,j}(\mu)$, $1 \leq j \leq N$

Note $a^q(\zeta^j, \zeta^i)$ $1 \leq i, j \leq N_{\max}$

$$\begin{aligned} &= a^q \left(\sum_{k=1}^{N_{\max}} \zeta_k^j \phi_k^{\text{FE}}, \sum_{k'=1}^{N_{\max}} \zeta_{k'}^i \phi_{k'}^{\text{FE}} \right) \\ &= \sum_{k=1}^{N_{\max}} \sum_{k'=1}^{N_{\max}} \zeta_k^j a^q(\phi_k^{\text{FE}}, \phi_{k'}^{\text{FE}}) \zeta_{k'}^i \\ &= \underline{\mathbf{Z}}_{N_{\max}}^T \underline{\mathbf{A}}^{\text{FE}, q} \underline{\mathbf{Z}}_{N_{\max}} . \end{aligned}$$

RB Approximation: Goal

For any $\varepsilon_{\text{des}} > 0$, evaluate

ACCURACY

$$\mu \in \mathcal{D} \rightarrow s_N^{\mathcal{N}}(\mu) \ (\approx s^{\mathcal{N}}(\mu))$$

that *provably* achieves desired accuracy

RELIABILITY

$$|s^{\mathcal{N}}(\mu) - s_N^{\mathcal{N}}(\mu)| \leq \varepsilon_{\text{des}}$$

but at (very low) marginal cost $\partial t_{\text{comp}}^{\dagger}$

EFFICIENCY

independent of \mathcal{N} as $\mathcal{N} \rightarrow \infty$.

[†] ∂t_{comp} : time to perform *one additional certified* evaluation $\mu \rightarrow s_N^{\mathcal{N}}(\mu)$.

RB Approximation: Goal

Real-Time Context (parameter estimation, ...):

$$t_0 : \mu \rightarrow t_0 + \partial t_{\text{comp}} : s_N^{\mathcal{N}}(\mu) .$$

"need" "response"

Many-Query Context (dynamic simulation, ...):

$$t_{\text{comp}}(\mu_j \rightarrow s_N^{\mathcal{N}}(\mu_j), j = 1, \dots, J)$$

$$= \partial t_{\text{comp}} J \text{ as } J \rightarrow \infty .$$

If we require

real-time evaluation $\mu \rightarrow s^{\mathcal{N}}(\mu)$

or

many evaluations $\mu^k \rightarrow s^{\mathcal{N}}(\mu^k), k = 1, \dots, \infty$

OFFLINE-ONLINE reduced-basis approximation

offers *order-of-magnitude* — N vs. \mathcal{N} — advantage.

Questions: Approximation

Can we develop *stable approximations*
for noncoercive and nonlinear problems? Y
[ST, HZ; NS]

Can we choose our *parameter samples*
 S_N ($\Rightarrow W_N$) wisely? ... adaptively? Y [Greedies]

Can we prove *exponential convergence*
 $u_N \rightarrow u^N$ uniformly[†] for all $\mu \in \mathcal{D}$? Y, BUT

ST = Stokes, HZ = Helmholtz, NS = Navier-Stokes problem
Greedy Algorithm: see ARCMCE review paper [RHP08], sect. 7

[†]Uniform (sharp) proofs available only for $P = 1$ parameter [MPT].

Questions: *A Posteriori* Error Estimation

Can we develop real-time $\times 2$

rigorous, sharp, efficient[†]

(Output) Error Bounds for

coercive problems? $\textcolor{red}{Y}[\text{SCM}, \alpha]$

noncoercive problems? $\textcolor{red}{Y}[\text{SCM}, \beta]$

(quadratically) nonlinear problems? $\textcolor{red}{Y}$

SCM = Successive Constraints Method (see ARCME review [RHP08], sect. 10)

[†]Efficiency equates to online complexity *independent of \mathcal{N}* .

Questions: Efficiency

Can we develop efficient

OFFLINE (\mathcal{N}) — ONLINE (N) Procedures

even for problems with

non-affine parameter (μ) dependence? Y, [EIM] †

non-polynomial “state” (u) dependence? Y, BUT †

EIM = Empirical Interpolation Method (CRAS [BMNP04])

M. Barrault, Y. Maday, N.C. Nguyen, A.T. Patera. An empirical interpolation method application to efficient reduced-basis discretization of partial differential equations. Comptes Rendus Mathematique, Analyse Numérique 2004, Vol 339, Pages 667-672

† In general, there will be some *loss of rigor* in our *a posteriori* error bounds.



Questions: Many Parameters

Can we consider *many* ($P \gg 1$)

“correlated” parameters[†]?

Y

independent parameters

of small variation?

Y

of large variation?

N

[†]For example, as in smooth shape/boundary optimization.

Questions: Domain Decomposition

Can we consider various

Domain Decomposition

approaches to improve

efficiency?

Y

generality?

Y [RBEM]

RBEM = Reduced Basis Element method and other options
(Hybrid RBHM, RDF, Static Condensation Method)

Maday, Ronquist, Lovgren, Nguyen, Patera, Eftang, Knezevic, Iapichino,
Quarteroni et al. ...

Reduced basis methods and a posteriori error estimation for parametrized PDEs

FUNDAMENTALS

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Course on Advanced Topics in Numerical Solution
of PDEs: Reduced Basis Methods for Computational Mechanics



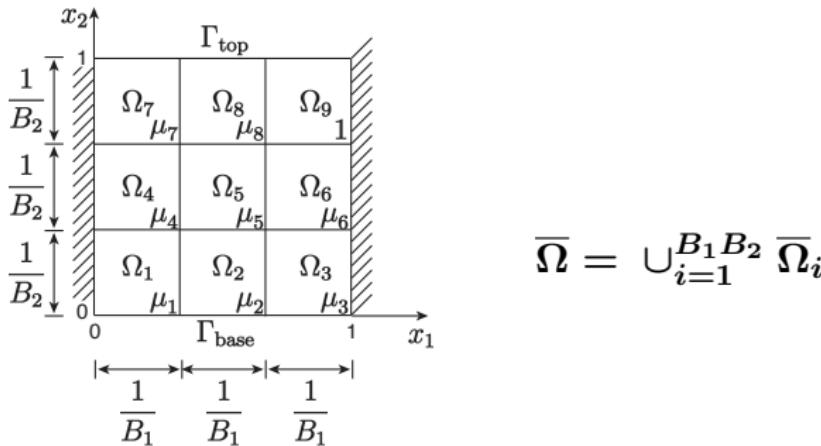
Example: Thermal Block

Given $\mu \equiv (\mu_1, \dots, \mu_P) \in \mathcal{D} \equiv [\mu^{\min}, \mu^{\max}]^P$ †

evaluate $s^e(\mu) = f(u^e(\mu))$

where $u^e(\mu) \in X^e \equiv \{v \in H^1(\Omega) \mid v|_{\Gamma_{\text{top}}} = 0\}$

satisfies $a(u^e(\mu), v; \mu) = f(v), \quad \forall v \in X^e.$



†Here $P = B_1 B_2 - 1$; we require $0 < \mu^{\min} < \mu^{\max} < \infty$.

Example: Thermal Block

Here

$$f(v) \equiv f^{\text{Neu}}(v) \equiv \int_{\Gamma_{\text{base}}} v ,$$

and

symmetric, coercive

$$a(w, v; \mu) = \sum_{i=1}^P \mu_i \int_{\Omega_i} \nabla w \cdot \nabla v + \int_{\Omega_{P+1}} \nabla w \cdot \nabla v ,$$

where $\overline{\Omega} = \cup_{i=1}^{P+1} \overline{\Omega}_i$.

Example: Thermal Block

We obtain

$$P = B_1 B_2 - 1$$

$$a(w, v; \mu) = \sum_{q=1}^{Q=P+1} \Theta^q(\mu) a^q(w, v)$$

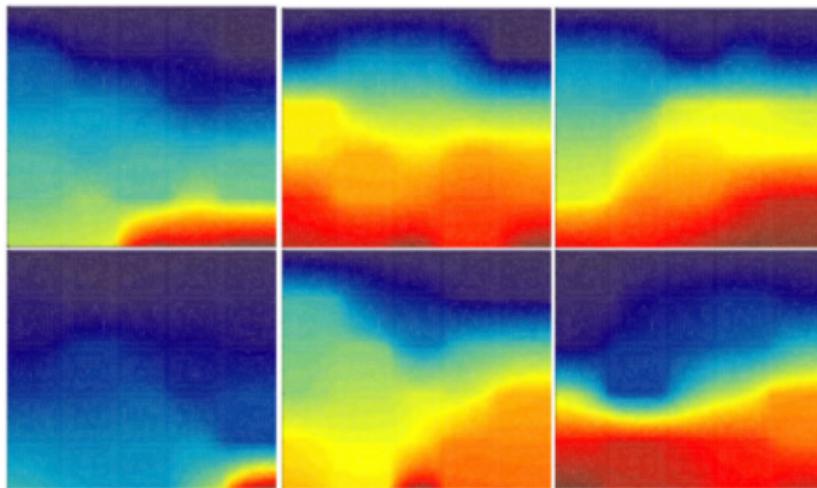
for

$$\Theta^q(\mu) = \mu_q, \quad 1 \leq q \leq P, \quad \text{and} \quad \Theta^{P+1} = 1 ,$$

and

$$a^q(w, v) = \int_{\Omega_q} \nabla w \cdot \nabla v, \quad 1 \leq q \leq P + 1 .$$

Example: Thermal Block



Representative Solutions

Sampling/Spaces Strategies: Preliminaries

Inner Products and Norms

Define, $\forall w, v \in X^e$

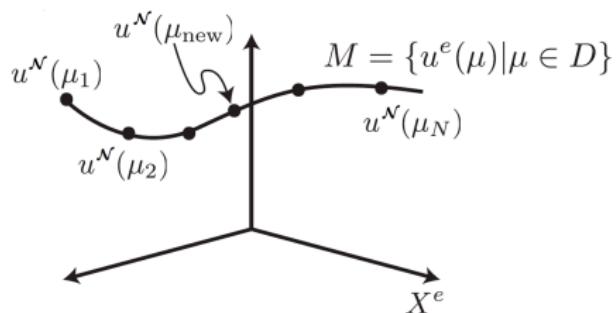
$$X^N \subset X^e$$

$$\left. \begin{aligned} ((w, v))_\mu &\equiv a(w, v; \mu) \\ |||w|||_\mu &\equiv ((w, w))_\mu^{1/2} \end{aligned} \right\} \text{energy}$$

and, given $\bar{\mu} \in \mathcal{D}$

$$\left. \begin{aligned} (w, v)_X &\equiv ((w, v))_{\bar{\mu}} + \tau(w, v)_{L^2(\Omega)} \\ \|w\|_X &\equiv (w, w)_X^{1/2} \end{aligned} \right\} X.$$

Sampling/Spaces Strategies: Preliminaries



\mathcal{M}^e = parameter-induced manifold
(low-Dimensional ($\mathcal{D} \subset \mathbb{R}^P$), very smooth)

Classical Approach

$X^{\mathcal{N}} \equiv \{v|_{T_h} \in \mathbf{IP}_I(T_h), \forall T_h \in \mathcal{T}_h\} \cap X^e; \dim(X^{\mathcal{N}}) \equiv \mathcal{N}.$

Reduced Basis Approach

$W_N \equiv \text{span}\{\zeta_n \equiv u^N(\mu_n), 1 \leq n \leq N\}$

Sampling/Spaces Strategies: Spaces

Nested Samples:

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

Hierarchical Spaces:

Lagrange

$$W_N^{\mathcal{N}} = \text{span}\{u^{\mathcal{N}}(\mu^n), \quad 1 \leq n \leq N\}, \quad 1 \leq N \leq N_{\max}.$$

Orthonormal Basis:

$$\{\zeta^{\mathcal{N}^n}\}_{1 \leq n \leq N_{\max}} = \mathbf{G}\cdot\mathbf{S} \left(\{u^{\mathcal{N}}(\mu^n)\}_{1 \leq n \leq N_{\max}}; (\cdot, \cdot)_X \right).$$

Sampling/Spaces Strategies: Gram-Schmidt Orthogonalization

Given $u^N(\mu^n)$, $1 \leq n \leq N_{\max}$:

Form $\{\zeta^n\}$, $1 \leq n \leq N_{\max}$ given as

$$n = 1, \zeta^1 = u^N(\mu^1) / \|u^N(\mu^1)\|_X;$$

for $n = 2: N_{\max}$

$$z^n = u^N(\mu^n) - \sum_{m=1}^{n-1} (u^N(\mu^n), \zeta^m)_X \zeta^m;$$

$$\zeta^n = z^n / \|z^n\|_X;$$

end.

As a result of this process we obtain the orthogonality condition

$$(\zeta^n, \zeta^m)_X = \delta_{nm}, \quad 1 \leq n, m \leq N_{\max}, \quad (1)$$

where δ_{nm} is the Kronecker-delta symbol

Sampling/Spaces Strategies: RB Galerkin Projection

Optimality:

$$|||u^N(\mu) - u_N^N(\mu)|||_\mu \leq \inf_{w \in W_N^N} |||u^N(\mu) - w|||_\mu ;$$

combination of snapshots.

Note also:

$$s^N(\mu) - s_N^N(\mu) \equiv |||u^N(\mu) - u_N^N(\mu)|||_\mu^2 ;$$

output converges as square.

Sampling/Spaces Strategies: RB Galerkin Projection

$$s^N(\mu) - s_N^N(\mu) \equiv |||u^N(\mu) - u_N^N(\mu)|||_{\mu}^2 ;$$

$$s^N(\mu) = f(u^N(\mu)); s_N^N(\mu) = f(u_N^N(\mu));$$

$$s^N(\mu) - s_N^N(\mu) = f(u^N(\mu)) - f(u_N^N(\mu)) =$$

$$= a(v, u^N(\mu) - u_N^N(\mu); \mu);$$

$$e(\mu) = u^N(\mu) - u_N^N(\mu);$$

$$a(v, e(\mu); \mu) = a(e(\mu), v; \mu) = a(e(\mu), e(\mu); \mu);$$

$$a(e(\mu), e(\mu); \mu) = |||u^N(\mu) - u_N^N(\mu)|||_{\mu}^2.$$

Sampling/Spaces Strategies: General “Reduced Model”

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

$$\text{evaluate } s_N^{\mathcal{N}}(\mu) = f(u_N^{\mathcal{N}}(\mu)) ,$$

where $u_N^{\mathcal{N}}(\mu) \in X_N^{\mathcal{N}} \subset X^{\mathcal{N}}$ satisfies $\dim(X_N^{\mathcal{N}}) = N$ [†]

$$a(u_N^{\mathcal{N}}(\mu), v; \mu) = f(v), \quad \forall v \in X_N^{\mathcal{N}} .$$

“Train” sample:

$$\Xi_{\text{train}} \subset \mathcal{D} \subset \mathbb{R}^P; \quad |\Xi_{\text{train}}| = n_{\text{train}} (\gg 1) .$$

“Test” sample:

$$\Xi_{\text{test}} \subset \mathcal{D} \subset \mathbb{R}^P; \quad |\Xi_{\text{test}}| = n_{\text{test}} (\gg 1) .$$

[†]Here $X_N^{\mathcal{N}}$ may be a hierarchical or non-hierarchical Lagrange ($W_N^{\mathcal{N}}$) or non-Lagrange RB space (Taylor, Hermite), or even a “non-RB” (non- $\mathcal{M}^{\mathcal{N}}$) space (Kolmogorov).

Sampling/Spaces Strategies: Norms

Given $\Xi \subset \mathcal{D}$, $y: \mathcal{D} \rightarrow \mathbb{R}$,

$$\|y\|_{L^\infty(\Xi)} \equiv \operatorname{ess\;sup}_{\mu \in \Xi} |y(\mu)| ,$$

$$\|y\|_{L^2(\Xi)} \equiv \left(|\Xi|^{-1} \sum_{\mu \in \Xi} y^2(\mu) \right)^{1/2} .$$

Given $z: \mathcal{D} \rightarrow X^{\mathcal{N}}$ (or X^e)

$$\|z\|_{L^\infty(\Xi; X)} \equiv \operatorname{ess\;sup}_{\mu \in \Xi} \|z(\mu)\|_X ,$$

$$\|z\|_{L^2(\Xi; X)} \equiv \left(|\Xi|^{-1} \sum_{\mu \in \Xi} \|z(\mu)\|_X^2 \right)^{1/2} .$$

Sampling/Spaces Strategies: 1. Lagrange “à la main”

Example: $P = 1$

$$\mathcal{D} \equiv [\mu^{\min}, \mu^{\max}]$$

$$S_N^{\text{nh,ln}} = \{\mu_N^n, 1 \leq n \leq N\}, \quad 1 \leq N \leq N_{\max},$$

$$\mu_N^n = \mu^{\min} \exp \left\{ \frac{n-1}{N-1} \ln \left(\frac{\mu^{\max}}{\mu^{\min}} \right) \right\}, \quad 1 \leq n \leq N;$$

$$W_N^{\mathcal{N} \text{ nh,ln}} = \text{span}\{u^{\mathcal{N}}(\mu_N^n), 1 \leq n \leq N\},$$

$$1 \leq N \leq N_{\max}.$$

[†]Note this Lagrange space is not hierarchical, and hence
not very practical; we denote non-hierarchical by “nh.”

Sampling/Spaces Strategies: 2. Proper Orthogonal Decomposition (POD)

Given Ξ_{train} ,

$$X_N^{\mathcal{N} \text{ POD}} = \arg \inf_{X_N^{\mathcal{N}} \subset \text{span}\{u^{\mathcal{N}}(\mu) \mid \mu \in \Xi_{\text{train}}\}} \|u^{\mathcal{N}} - \Pi_{X_N^{\mathcal{N}}} u^{\mathcal{N}}\|_{L^2(\Xi_{\text{train}}; X)} ;$$

eigenproblem interpretation demonstrates

hierarchical property.

Issues: \$\$ — n_{train} FE solutions,
 $n_{\text{train}} \times n_{\text{train}}$ eigenproblem;
weaker norm over Ξ_{train} .

ARCME review paper [RHP08], section 7

Sampling/Spaces Strategies: 2. POD

$\underline{C}^{POD} \in \mathbb{R}^{n_{\text{train}} \times n_{\text{train}}} : \text{ for } 1 \leq i, j \leq n_{\text{train}}$,

$$C_{ij}^{POD} = \frac{1}{n_{\text{train}}} \left(u(\mu_{\text{train}}^i), u(\mu_{\text{train}}^j) \right)_X,$$

Eigenpairs:

$(\underline{\psi}^{POD,k} \in \mathbb{R}^{n_{\text{train}}}, \lambda^{POD,k} \in \mathbb{R}_{+0}), 1 \leq k \leq n_{\text{train}},$

$$\underline{C}^{POD} \underline{\psi}^{POD,k} = \lambda^{POD,k} \underline{\psi}^{POD,k}.$$

Arranging eigenvalues in *descending* order:

$$\lambda^{POD,1} \geq \lambda^{POD,2} \geq \dots \lambda^{POD,n_{\text{train}}} \geq 0.$$

We now identify $\Psi^{POD,k} \in X, 1 \leq k \leq n_{\text{train}}$, as

$$\Psi^{POD,k} \equiv \sum_{m=1}^{n_{\text{train}}} \psi_m^{POD,k} u(\mu_{\text{train}}^m);$$

Sampling/Spaces Strategies: 2. POD

Define N_{\max} as the smallest N such that

$$\left(\bar{\varepsilon}_N^{POD} \equiv \right) \sqrt{\sum_{k=N+1}^{n_{\text{train}}} \lambda^{POD,k}} \leq \varepsilon_{tol,\min} .$$

POD RB spaces

$$X_N^{POD} = \text{span}\{\Psi^{POD,n}, 1 \leq n \leq N\}, \quad 1 \leq N \leq N_{\max} ;$$

$$(\Psi^{POD,n}, \Psi^{POD,m})_X = \delta_{nm}, 1 \leq n, m \leq n_{\text{train}}$$

and hence $(\Psi^{POD,n} \equiv) \xi^n = \zeta^n, 1 \leq n \leq N_{\max}$.

Sampling/Spaces Strategies: 3. Greedy Algorithm

Given Ξ_{train} , $S_1 = \{\mu^1\}$, $W_1^N = \text{span}\{u^N(\mu^1)\}$,
 [for $N = 2, \dots, N_{\max}$:

$$\begin{aligned}\mu^N &= \arg \max_{\mu \in \Xi_{\text{train}}} \Delta_{N-1}(\mu) \\ S_N &= S_{N-1} \cup \mu^N; \\ W_N^N &= W_{N-1}^N + \text{span}\{u^N(\mu^N)\}.\end{aligned}$$

Issue: suboptimal (heuristic).

Here, for $N = 1, \dots$

$$\|u^N(\mu) - u_{W_N^N}^N(\mu)\|_X \leq \Delta_N(\mu), \quad \forall \mu \in \mathcal{D}:$$

$\Delta_N(\mu)$ is a sharp, *inexpensive*[†] *a posteriori* error bound for
 $\|u^N(\mu) - u_{W_N^N}^N(\mu)\|_X$.

Greedy only computes actual (*winning* candidate) snapshots.

[†]Marginal cost (= average asymptotic cost) is *independent* of N .

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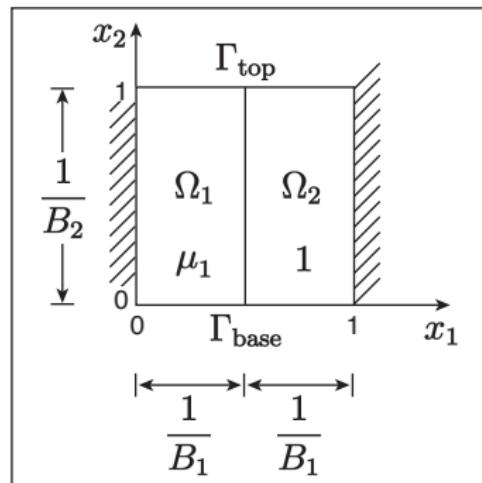
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Convergence: $P = 1$

Example: Thermal Block — (2, 1)



Geometry

Convergence: $P = 1$

Problem statement

Given $\mu = (\mu_1) \in \mathcal{D} \equiv [\mu^{\min}, \mu^{\max}]$,

evaluate $s^e(\mu) = f(u^e(\mu))$

where $u^e(\mu) \in X^e \equiv \{v \in H^1(\Omega) \mid v|_{\Gamma_{\text{top}}} = 0\}$

satisfies $a(u^e(\mu), v; \mu) = f(v), \quad \forall v \in X^e.$

Choose $\mu_{\min} = \frac{1}{\sqrt{\mu_r}}$, $\mu_{\max} = \sqrt{\mu_r}$ ($\frac{\mu_{\max}}{\mu_{\min}} = \mu_r$); $\mu_r = 100$.

Convergence: $P = 1$

Problem statement

Here

$(Q = 2)$

$$f \left(= f^{\text{Neu}}(v) = \int_{\Gamma_{\text{base}}} v, \forall v \in X^e \right) \in (X^e)'$$

and

$$a(w, v; \mu) = \mu \int_{\Omega_1} \nabla w \cdot \nabla v + \int_{\Omega_2} \nabla w \cdot \nabla v ,$$

where $\overline{\Omega} = \overline{\Omega}_1 \cup \overline{\Omega}_2$.

Convergence: $P = 1$

FE Approximation

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

$\mathcal{N} = 1024^\dagger$

evaluate $s^{\mathcal{N}}(\mu) = f(u^{\mathcal{N}}(\mu))$,

where $u^{\mathcal{N}}(\mu) \in X^{\mathcal{N}} \subset X^e$ satisfies

$a(u^{\mathcal{N}}(\mu), v; \mu) = f(v), \quad \forall v \in X^{\mathcal{N}}$.

[†]Note here $\text{span}\{\mathcal{M}^{\mathcal{N}}\}$ is of dimension $\approx 4\sqrt{\mathcal{N}}$.

Convergence: $P = 1$

RB Approximation

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

$$\text{evaluate } s_N^{\mathcal{N}}(\mu) = f(u_N^{\mathcal{N}}(\mu)) ,$$

where $u_N^{\mathcal{N}}(\mu) \in X_N^{\mathcal{N}} \subset X^{\mathcal{N}}$ satisfies $\dim(X_N^{\mathcal{N}}) = N$ [†]

$$a(u_N^{\mathcal{N}}(\mu), v; \mu) = f(v), \quad \forall v \in X_N^{\mathcal{N}} .$$

[†]In Lagrange case, $X_N^{\mathcal{N}} = W_N^{\mathcal{N}}$ (hierarchical) or $W_N^{\mathcal{N} \text{ nh}}$ (non-hierarchical).

Convergence: $P = 1$

A *Priori* Theory [Maday, Patera and Turinici, ..., PR book]

Choose (non-hierarchical)

$$S_N^{\text{nh,ln}} = \{\mu_N^n, 1 \leq n \leq N\}, \quad 1 \leq N \leq N_{\max},$$

$$\mu_N^n = \mu^{\min} \exp \left\{ \frac{n-1}{N-1} \ln \left(\frac{\mu^{\max}}{\mu^{\min}} \right) \right\}, \quad 1 \leq n \leq N;$$

$$W_N^{\mathcal{N} \text{ nh,ln}} = \text{span}\{u^{\mathcal{N}}(\mu_N^n), 1 \leq n \leq N\}, \quad 1 \leq N \leq N_{\max}.$$

Proposition 1

For any $f \in (X^e)'$, $N \geq 2$

$$\frac{\|u^{\mathcal{N}}(\mu) - u_N^{\mathcal{N}}(\mu)\|_{\mu}}{\|u^{\mathcal{N}}(\mu)\|_{\mu}} \leq \exp \left\{ - \frac{N-1}{N_{\text{crit}}-1} \right\}, \quad \forall \mu \in \mathcal{D}$$

for $N \geq N_{\text{crit}} = 1 + [2e \ln \mu_r]_+$. □

Note "no" dependence on spatial regularity; "no" dependence on \mathcal{N} ; weak dependence on μ .

Convergence: $P = 1$

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Note "no" dependence on spatial regularity; "no" dependence on \mathcal{N} ; weak dependence on μ_r .

Convergence: $P = 1$

Algorithms

Recall Greedy *heuristically* minimizes

RB error *bound* in $L^\infty(\Xi_{\text{train}}; X)$,

while POD *truly* minimizes

projection error in $L^2(\Xi_{\text{train}}; X)$;

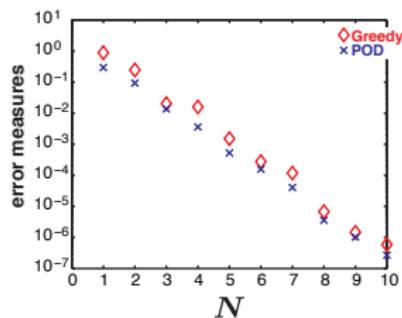
further recall

Cost (Greedy) \ll Cost (POD) for large n_{train} .

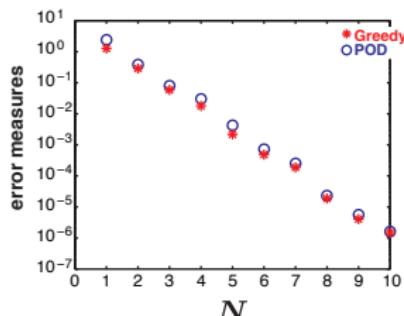
Convergence: $P = 1$

Numerical Results

$$\|u^N - u_N^N\|_{L^2(\Xi; X)}$$

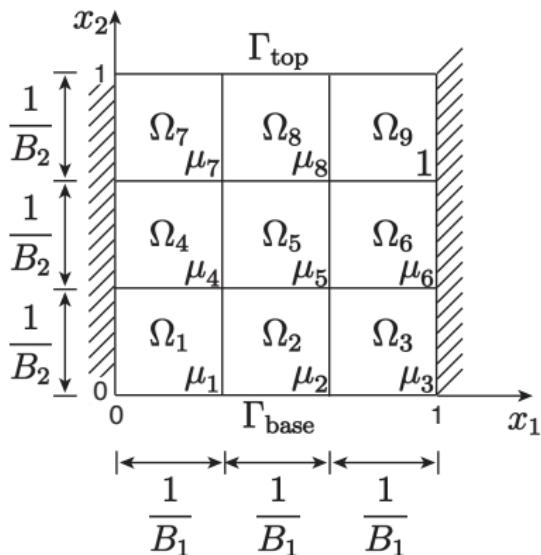


$$\|u^N - u_N^N\|_{L^\infty(\Xi; X)}$$



Convergence: $P > 1$

Example: Thermal Block — (3, 3)



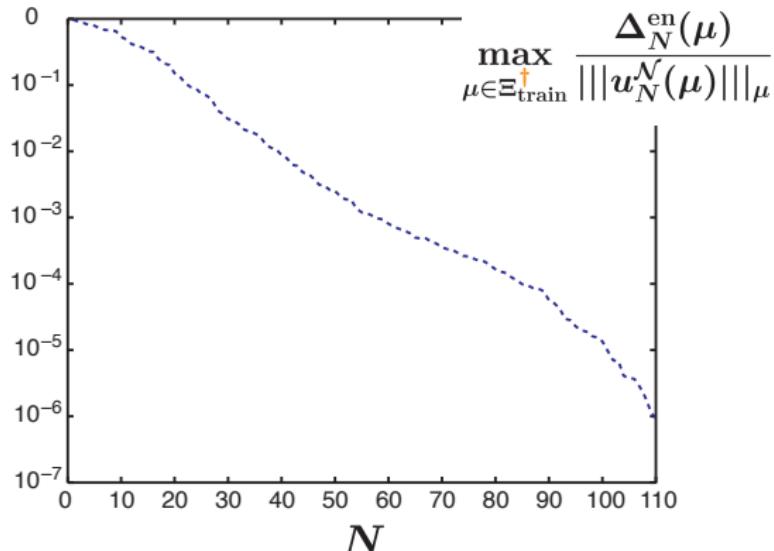
$$\overline{\Omega} = \bigcup_{i=1}^{B_1 B_2} \overline{\Omega}_i$$

Geometry

Convergence: $P > 1$

Example: Thermal Block — (3, 3)

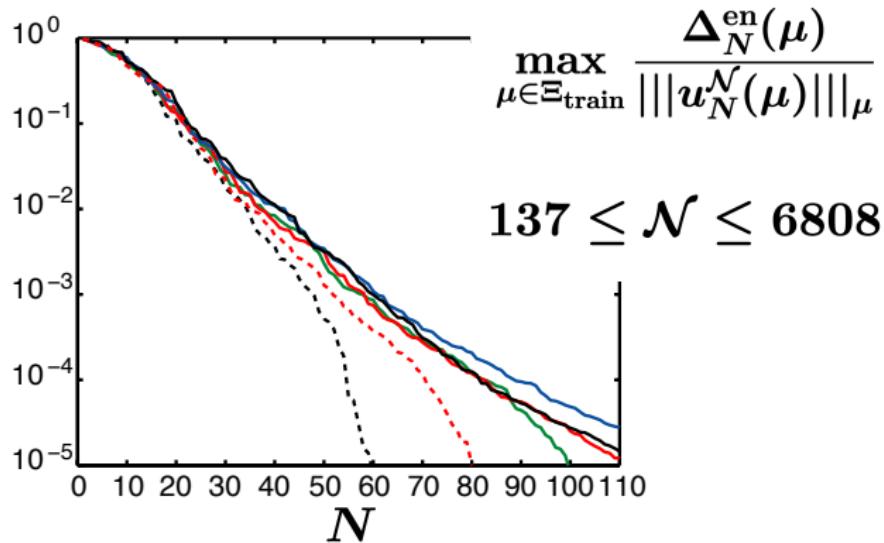
Greedy: RB Energy Error



[†]Here Ξ_{train} is a Monte Carlo sample in $\ln \mu$ of size $n_{\text{train}} = 5000$ ($\gg N$); note $|||u^N(\mu) - u_N^N(\mu)|||_\mu \leq \Delta_N^{\text{en}}(\mu)$, $|||u_N^N(\mu)|||_\mu \leq |||u^N(\mu)|||_\mu$.

Convergence: $P > 1$

Example: Thermal Block — (3, 3)

Effect of X^N 

Reduced basis methods and a posteriori error estimation for parametrized PDEs

WORKED PROBLEMS

Gianluigi Rozza

Course on Advanced Topics in Numerical Solution
of PDEs: Reduced Basis Methods for Computational Mechanics



Problem "Scope": Geometry

Domain decomposition: definition

Original Domain $\Omega_o(\mu)$,

$$u_o^e \in X_o^e(\Omega_o(\mu))$$

$$\overline{\Omega}_o(\mu) = \bigcup_{k=1}^{K_{\text{dom}}} \overline{\Omega}_o^k(\mu);$$

Reference domain Ω ,

$$u^e \in X^e(\Omega)$$

$$\overline{\Omega} = \bigcup_{k=1}^{K_{\text{dom}}} \overline{\Omega}^k,$$
common configuration

where $\Omega = \Omega_o(\mu_{\text{ref}})$ for $\mu_{\text{ref}} \subset \mathcal{D}^\dagger$.

For Ω^k , $\Omega_o^k(\mu)$ we choose in \mathbf{R}^2 triangles, elliptical triangles and curvy triangles. In \mathbf{R}^3 we choose parallelepipeds (and in theory tetrahedra). Other more standard options are available to be treated "by hand".

[†]Connectivity requirement: subdomain intersections

must be an entire edge, a vertex, or null.

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Affine Mappings

Require

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

$$\overline{\Omega}_o^k(\mu) = \mathcal{T}^{\text{aff},k}(\overline{\Omega}^k; \mu), \quad 1 \leq k \leq K_{\text{dom}},$$

where

$$\mathcal{T}^{\text{aff},k}(x; \mu) = C^{\text{aff},k}(\mu) + G^{\text{aff},k}(\mu)x,$$

is an invertible affine mapping from $\overline{\Omega}^k$ onto $\overline{\Omega}_o^k(\mu)$.

Further require

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

$$\mathcal{T}^{\text{aff},k}(x; \mu) = \mathcal{T}^{\text{aff},k'}(x; \mu), \quad \forall x \in \overline{\Omega}^k \cap \overline{\Omega}^{k'}, \\ 1 \leq k, k' \leq K_{\text{dom}},$$

to ensure a *continuous* piecewise-affine global mapping $\mathcal{T}^{\text{aff}}(\cdot; \mu)$ from $\overline{\Omega}$ onto $\overline{\Omega}_o(\mu)$.[†]

[†]It follows that for $w_o \in H^1(\overline{\Omega}_o(\mu))$, $w_o \circ \mathcal{T}^{\text{aff}} \in H^1(\Omega)$.



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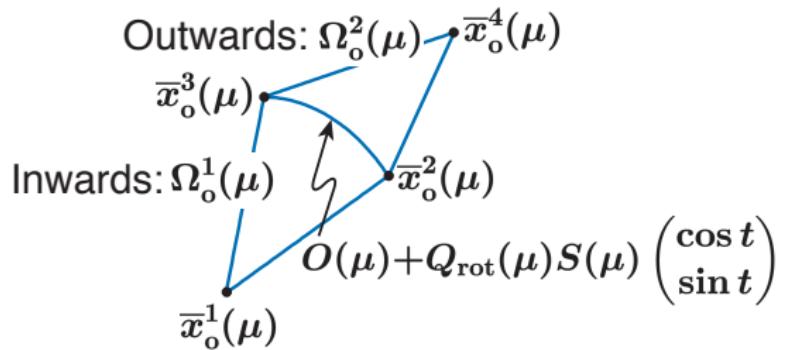
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Affine Mappings

Elliptical Triangles: definition



$$O(\mu) = (x_{o1}^{\text{cen}}, x_{o2}^{\text{cen}})^T$$

$$Q_{\text{rot}}(\mu) = \begin{pmatrix} \cos \phi(\mu) & -\sin \phi(\mu) \\ \sin \phi(\mu) & \cos \phi(\mu) \end{pmatrix}$$

$$S(\mu) = \text{diag}(\rho_1(\mu), \rho_2(\mu))$$

Affine Mappings

Elliptical Triangles: constraints

Given $\bar{x}_o^2(\mu), \bar{x}_o^3(\mu)$, find $\bar{x}_o^1(\mu), \bar{x}_o^4(\mu)$ $(\Rightarrow \mathcal{T}^{\text{aff},1\&2})$

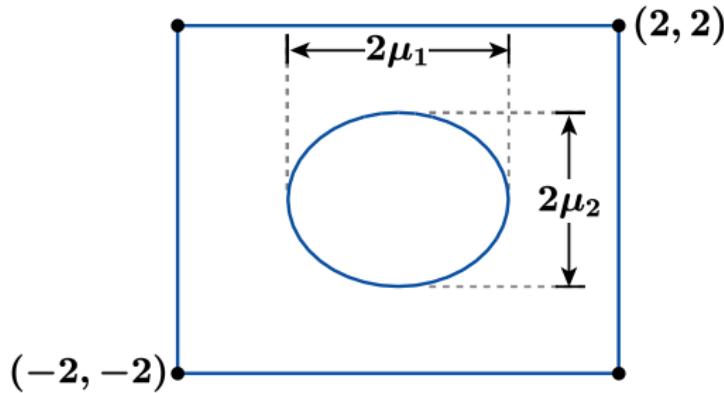
- $$\left. \begin{array}{l} (i) \quad \text{produce desired elliptical arc} \\ (ii) \quad \text{satisfy internal angle criterion} \end{array} \right\} \forall \mu \in \mathcal{D};$$

these conditions ensure *continuous invertible* mappings.

[†]Explicit recipes for admissible $x_o^1(\mu)$ (Inwards case)
and $x_o^4(\mu)$ (Outwards case) are readily obtained.

Affine Mappings

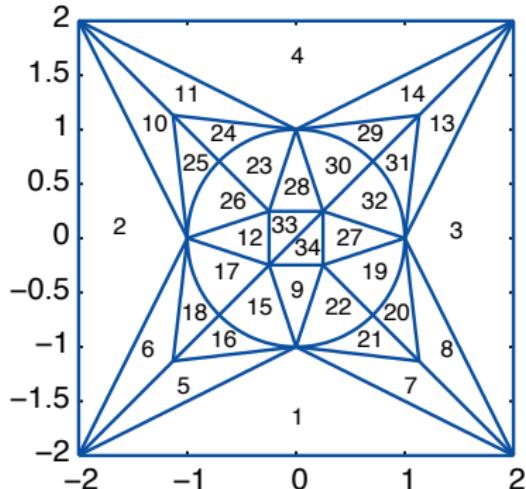
Elliptical Triangles: example (CinS triangulation)



$$\Omega_o(\mu): \mu = (\mu_1, \mu_2, \dots) \subset \mathcal{D} \equiv [0.8, 1.2]^2 \times \dots$$

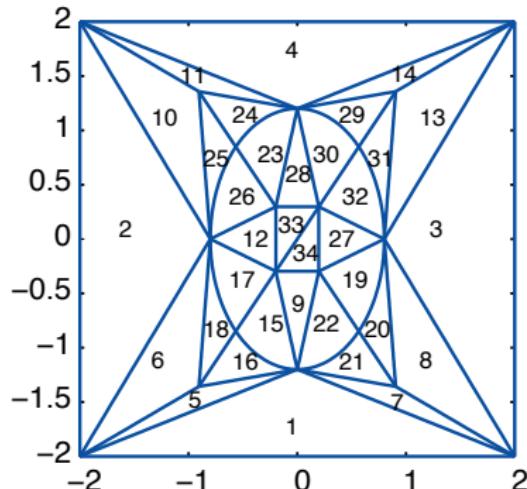
Affine Mappings

Elliptical Triangles: example (CinS triangulation)



$$\Omega = \Omega_o(\mu_{\text{ref}} = (1, 1))$$

(C) rbMIT



$$\Omega_o(\mu = (0.8, 1.2))$$

Affine Mappings

Curvy Triangles: definition

Outwards: $\Omega_o^2(\mu) \rightarrow \bar{x}_o^4(\mu)$

Inwards: $\Omega_o^1(\mu) \rightarrow \bar{x}_o^3(\mu)$

$O(\mu) + Q_{\text{rot}}(\mu) S(\mu) \begin{pmatrix} g_1(t) \\ g_2(t) \end{pmatrix}$

$$\overbrace{O(\mu) = (x_{o1}^{\text{cen}}, x_{o2}^{\text{cen}})^T}^{(x_{o1}^{\text{cen}}, x_{o2}^{\text{cen}})^T}$$

$$Q_{\text{rot}}(\mu) = \begin{pmatrix} \cos \phi(\mu) & -\sin \phi(\mu) \\ \sin \phi(\mu) & \cos \phi(\mu) \end{pmatrix}$$

$$S(\mu) = \text{diag}(\rho_1(\mu), \rho_2(\mu))$$

Affine Mappings

Curvy Triangles: constraints

Given $\bar{x}_o^2(\mu), \bar{x}_o^3(\mu)$, find $\bar{x}_o^1(\mu), \bar{x}_o^4(\mu)$ $(\Rightarrow \mathcal{T}^{\text{aff},1\&2})$

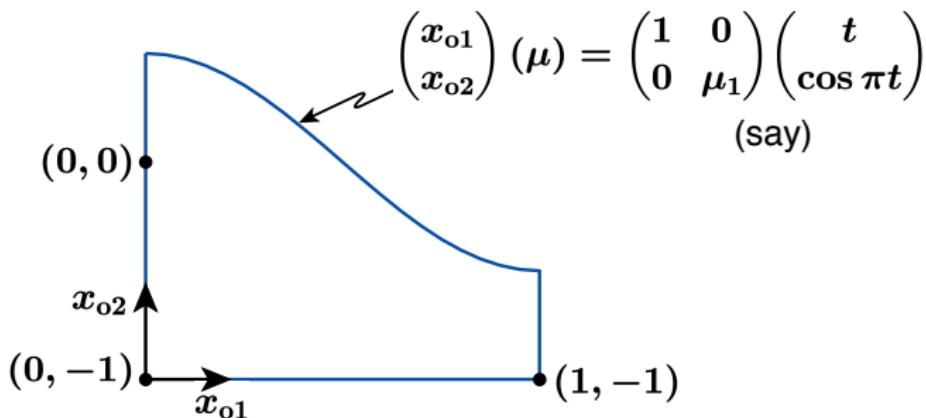
- $$\left. \begin{array}{l} (i) \quad \text{produce desired curvy arc} \\ (ii) \quad \text{satisfy internal angle criterion} \end{array} \right\} \forall \mu \in \mathcal{D};$$

these conditions ensure *continuous invertible* mappings.

[†]Quasi-explicit recipes for admissible $\bar{x}_o^1(\mu)$ and $\bar{x}_o^4(\mu)$ can (sometimes) be obtained in the convex/concave case.

Affine Mappings

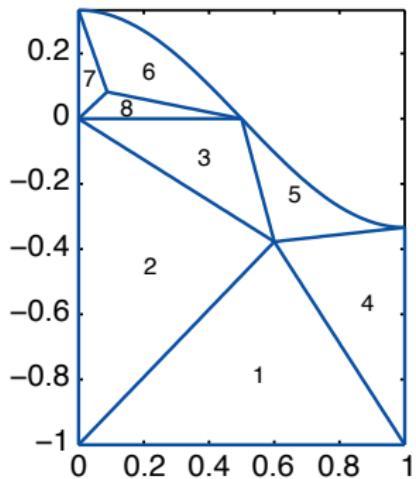
Elliptical Triangles: example (Cosine triangulation)



$$\Omega_o(\mu): \mu = (\mu_1, \dots) \subset \mathcal{D} \equiv [\frac{1}{6}, \frac{1}{2}] \times \dots$$

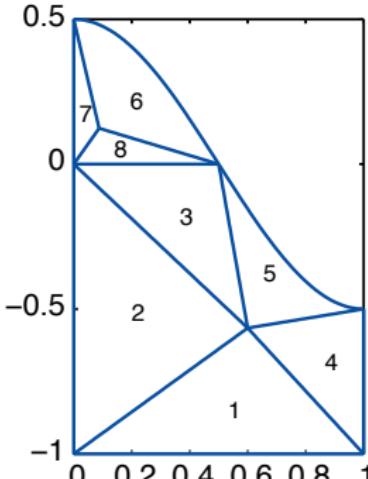
Affine Mappings

Elliptical Triangles: example (Cosine triangulation)



$$\Omega = \Omega_o (\mu_{\text{ref}} = \frac{1}{3})$$

(C) rbMIT



$$\Omega_o (\mu = \frac{1}{2})$$

Problem Scope: Bilinear Form

Transformation: Formulation on original domain (\mathbb{R}^2)

$$\text{For } w, v \in H^1(\Omega_o(\mu))^\dagger \quad u_o^e(\mu) \in H_0^1(\Omega_o(\mu))$$

$$a_o(w, v; \mu) = \sum_{k=1}^{K_{\text{dom}}} \int_{\Omega_o^k(\mu)} \begin{bmatrix} \frac{\partial w}{\partial x_{o1}} & \frac{\partial w}{\partial x_{o2}} & w \end{bmatrix} \mathcal{K}_{oij}^k(\mu) \begin{bmatrix} \frac{\partial v}{\partial x_{o1}} \\ \frac{\partial v}{\partial x_{o2}} \\ v \end{bmatrix}$$

where $\mathcal{K}_o^k: \mathcal{D} \rightarrow \mathbf{R}^{3 \times 3}$, SPD for $1 \leq k \leq K_{\text{dom}}$

(note \mathcal{K}_o^k affine in x_o is also permissible).

[†] We consider the scalar case; the vector case (linear elasticity) admits an analogous treatment.

Problem Scope: Bilinear Form

Transformation: Formulation on reference domain

$$\text{For } w, v \in H^1(\Omega) \quad u^e(\mu) \in H_0^1(\Omega)$$

$$a(w, v; \mu) = \sum_{k=1}^{K_{\text{dom}}} \int_{\Omega^k} \begin{bmatrix} \frac{\partial w}{\partial x_1} & \frac{\partial w}{\partial x_2} & w \end{bmatrix} \mathcal{K}_{ij}^k(\mu) \begin{bmatrix} \frac{\partial v}{\partial x_1} \\ \frac{\partial v}{\partial x_2} \\ v \end{bmatrix}$$

$$\mathcal{K}^k(\mu) = |\det G^{\text{aff}, k}(\mu)| D(\mu) \mathcal{K}_o^k(\mu) D^T(\mu), \text{ and}$$

$$D(\mu) = \begin{pmatrix} (G^{\text{aff}, k})^{-1} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

ARCME [RHP08], section 5

Problem Scope: Bilinear Form

Transformation: Affine form

Expand

$$a(w, v; \mu) = \underbrace{\mathcal{K}_{11}^1(\mu)}_{\Theta^1(\mu)} \underbrace{\int_{\Omega^1} \frac{\partial w}{\partial x_1} \frac{\partial v}{\partial x_1}}_{a^1(w, v)} + \dots$$

with as many as $Q = 4K$ terms.

We can often greatly reduce the requisite Q .

Achtung! Many interesting problems are **not** affine (or require Q very large).

For example, $\mathcal{K}_o^k(x; \mu)$ for general x dependence; and nonzero Neumann conditions on curvy $\partial\Omega$ yields non-affine $a(\cdot, \cdot; \mu)$.

Problem Scope: Bilinear Form

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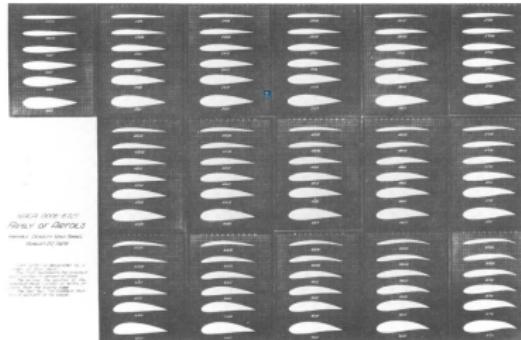
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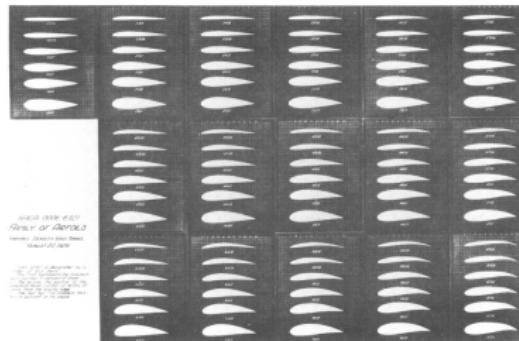
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Flow around parametrized airfoils



- Flow simulation around different airfoils within a NACA family
- evaluation of the airfoil performance (pressure coefficient)

Flow around parametrized airfoils



- Flow simulation around different airfoils within a NACA family
- evaluation of the airfoil performance (pressure coefficient)

Affine mappings based on domain decomposition and boundary parametrization

$$\mathbf{x}_o = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} \cos \mu_2 & -\sin \mu_2 \\ \sin \mu_2 & \cos \mu_2 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & \pm \mu_1/20 \end{pmatrix} \begin{pmatrix} 1-t^2 \\ \varphi(t) \end{pmatrix}, \quad t \in [0, \sqrt{0.3}]$$

$$\mathbf{x}_o = \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \begin{pmatrix} \cos \mu_2 & -\sin \mu_2 \\ \sin \mu_2 & \cos \mu_2 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \pm \mu_1/20 \end{pmatrix} \begin{pmatrix} t^2 \\ \varphi(t) \end{pmatrix}, \quad t \in [\sqrt{0.3}, 1],$$

$$\varphi(t) = 0.2969t - 0.1260t^2 - 0.3520t^4 + 0.2832t^6 - 0.1021t^8$$

$$\text{thickness } \mu_1 \in [4, 24], \quad \text{angle of attack } \mu_2 \in [0, \pi/4]$$

Flow around parametrized airfoils

Laplace equation(velocity potential):

$$\begin{aligned} -\Delta\phi &= 0 && \text{in } \Omega_o(\mu) \\ \frac{\partial\phi}{\partial\mathbf{n}} &= 0 && \text{on } \Gamma_w(\mu) \\ \frac{\partial\phi}{\partial\mathbf{n}} &= \phi_{in} && \text{on } \Gamma_{in}(\mu) \\ \phi &= \phi_{ref} && \text{on } \Gamma_{out}(\mu), \end{aligned}$$

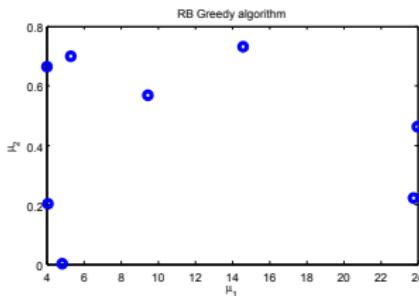
Pressure and velocity:

$$\mathbf{v} = \nabla\phi$$

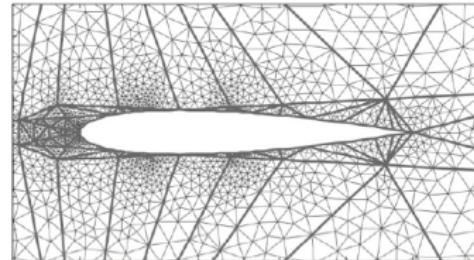
$$p + \frac{1}{2}\rho|u|^2 = p_{in} + \frac{1}{2}\rho|v_{in}|^2, \quad \text{in } \Omega_o(\mu),$$

Pressure coefficient

$$c_p(p) = \frac{p - p_{in}}{\frac{1}{2}\rho|u_{in}|^2} = 1 - \left(\frac{|u|^2}{|u_{in}|^2} \right),$$

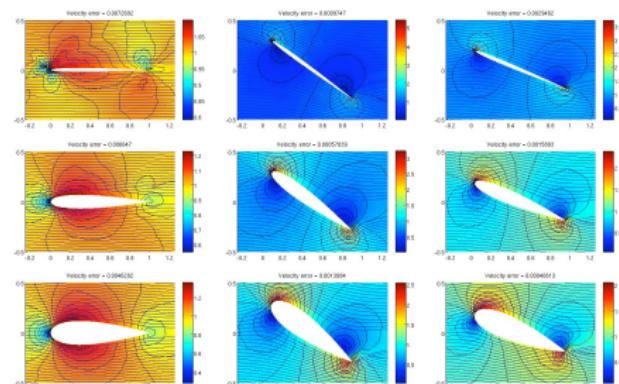
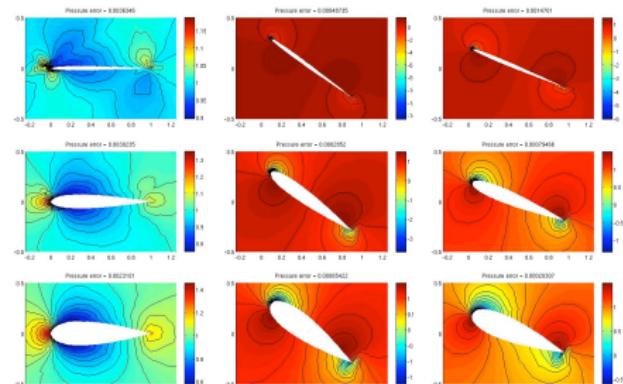


Greedy sampling (parameter space)



Automatic affine maps + domain decomposition

Flow around parametrized airfoils



Number of FE dof \mathcal{N}

$\approx 3,500$

Number of RB basis functions N

8

Automatic affine domain decomposition

$$t_{FE}^{offline} = 8h$$

Greedy algorithm + RB structures/space

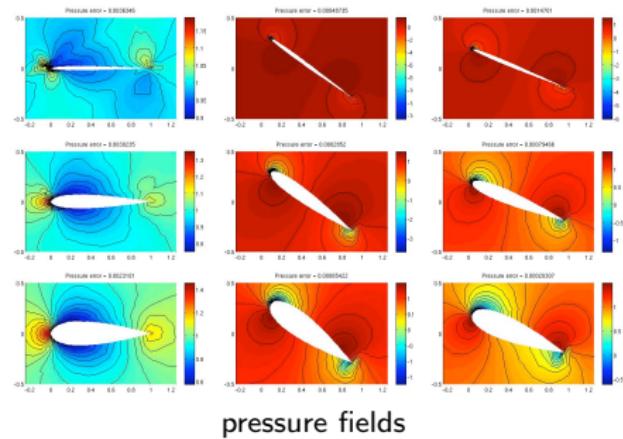
$$t_{RB}^{offline} = 4h$$

Computational speedup

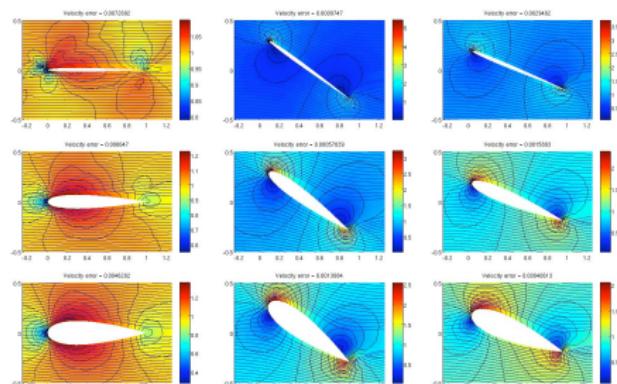
$$t_{RB}^{online} / t_{FE}^{online} = 250^3$$

³Computations carried out on a single processor of a 2GHz Dual Core AMD Opteron(tm) processor 2214 HE and 16 GB of RAM

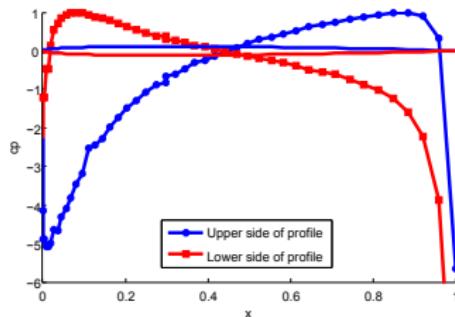
Flow around parametrized airfoils



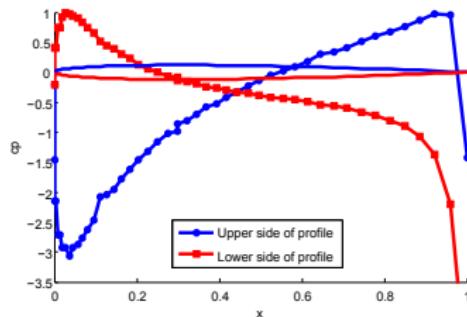
pressure fields



velocity fields



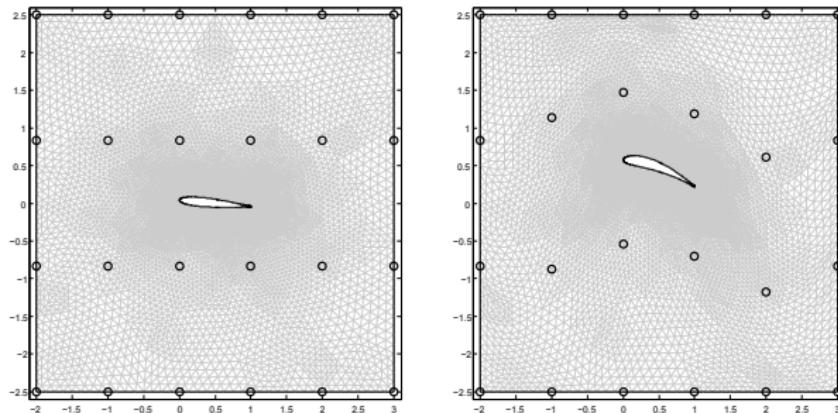
Pressure coefficients for two different NACA airfoils



Flow around parametrized airfoils

Other possible options

FFD



RBF

