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(Joint work with Claudio Canuto, Karsten Urban)

A-Posteriori Error Estimators for RBM Applied to Quadratic Non-Linear PPDEs (Involving Non-Affine Coefficient Functions)

Motivation

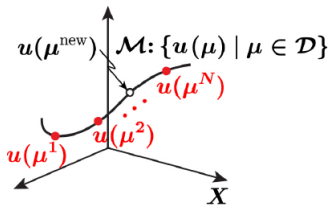
- Reduced-Basis Methods
- Application

Theory

- Problem
 - Primal Problem
 - Dual Problem
 - Existence, Uniqueness and Well-Posedness
- A-Posteriori Error Estimation

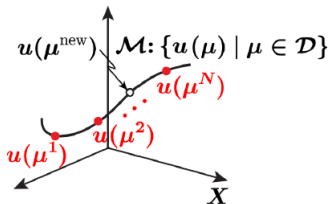
Numerical Results

Reduced-Basis Methods for solving PPDEs **rapidly**, **repeatedly** and **reliably**.

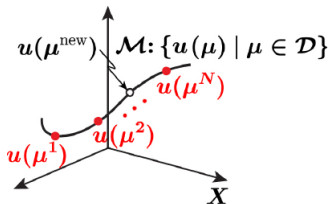


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- Usage of N **global** basis functions $\xi_n := u(\mu_n)$, $N \ll \mathcal{N} := \dim(X)$ is sufficient.

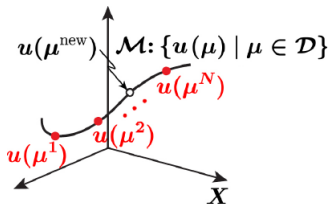


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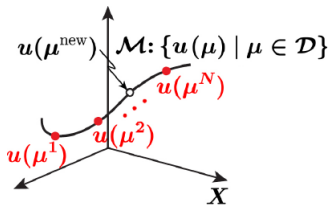
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- Availability of **a-posteriori error estimators**
 1. ensures reliability;
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- Efficient treatment of **output functionals**.
- **Offline/Online Decomposition** allows for a \mathcal{N} -independent online-stage.

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Compute

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- $\xi_i = \frac{1}{\sqrt{\lambda_i}} \sum_{j=1}^n (v_i)_j u_j$, $1 \leq i \leq N$, where λ_i is the i -th largest eigenvalue of K and v_i is the corresponding eigenvector.

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Then, it is proven that

1. $(\xi_i, \xi_j)_X = \delta_{ij}$, $1 \leq i, j \leq n$ and
2. $\int_{\mathcal{D}} \left\| u(\mu) - \sum_{i=1}^N (u(\mu), \xi_i)_X \xi_i \right\|_X^2 d\mu = \sum_{i=N+1}^n \lambda_i$.

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Then for $N = 1, 2, \dots$

1. compute

$$\mu^* := \arg \max_{\mu \in \Xi} \Delta(\mu);$$

2. if $\Delta(\mu^*) > \varepsilon$, update $S^{N+1} := S^N \cup \{\mu^*\}$ and continue;

3. stop,

where $\Delta(\mu)$ is a **rapidly evaluable, reliable a-posteriori** error estimator for $\|u(\mu) - \hat{u}(\mu)\|_X$.

Application

For $\mu \in \mathcal{D} := [0, \frac{\pi}{2}]$ we aim in solving

$$\begin{cases} -a\Delta u + (\underline{b} \cdot \nabla u) u + cu^2 = 0, & \text{in } \Omega(\mu), \\ u = 0, & \text{on } \partial B(\mu), \\ u = g, & \text{on } \Gamma_D, \\ \frac{\partial u}{\partial n} = 0, & \text{on } \Gamma_N. \end{cases}$$

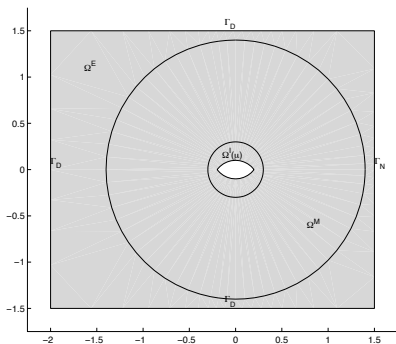


Figure: Geometry for one blade.

Mapping to a **reference situation** yields:

Find $\check{u}(\mu) \in u_0 + X$, s.t. $\forall \check{v} \in X$:

$$\int_{\check{\Omega}} (\underline{\underline{\alpha}}(\cdot; \mu) \nabla \check{u}) \cdot \nabla \check{v} \, d\check{\Omega} + \int_{\check{\Omega}} (\underline{\underline{\beta}}(\cdot; \mu) \cdot \nabla \check{u}) \check{u} \check{v} \, d\check{\Omega} + \int_{\check{\Omega}} \gamma(\cdot; \mu) \check{u}^2 \check{v} \, d\check{\Omega} = 0,$$

where

- $X := \{v \in H^1(\check{\Omega}) : v = 0 \text{ on } \Gamma_D \cup \partial\check{B}\}$;
- $u_0 \in H^1(\Omega_E) : u_0 = g \text{ on } \Gamma_D, u_0 = 0 \text{ on } \partial\Omega_E \setminus \Gamma_D$.

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Primal Problem (Generalization of [?]) (K. Veroy, A.T. Patera; 2005):

$$\left\{ \begin{array}{l} \text{For } \mu \in \mathcal{D} \subset \mathbb{R}^p \text{ find } u(\mu) \in X, \text{ s.t. for all } v \in X: \\ g(u(\mu), v; h(\mu)) := a(u(\mu), v; h_a(\mu)) + b(u(\mu), u(\mu), v; h_b(\mu)) - f(v) = 0, \end{array} \right.$$

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where

- $\Omega \subset \mathbb{R}^n$, $X \subset X^e \subset H^1(\Omega)$;
- $h(\mu) := \{h_a(\mu), h_b(\mu)\}$, $h_i(\mu) := h_i(\cdot; \mu)$, $h_i \in L^\infty(\Omega) \times C^1(\mathcal{D})$;
- $a(w, v; h_a)$ is linear in $w, v \in X$ and $h_a \in L^\infty(\Omega)$;
- $b(w, z, v; h_b)$ is linear in $w, z, v \in X$ and $h_b \in L^\infty(\Omega)$;
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Output of Interest:

- $s(\mu) := \ell(u(\mu))$, where ℓ is a bounded, linear functional in X .

Frechét derivative $dg(\cdot, \cdot; h)[z] : X \times X \rightarrow \mathbb{R}$ at $z \in X$ is

$$dg(w, v; h)[z] := a(w, v; h_a) + \underbrace{b(w, z, v; h_b) + b(z, w, v; h_b)}_{=: db(w, v; h_b)[z]}.$$

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Inf-sup parameter and **continuity constant** (for fixed $z \in X$):

$$\beta(z; h) := \inf_{w \in X} \sup_{v \in X} \frac{dg(w, v; h)[z]}{\|w\|_X \|v\|_X},$$

$$\gamma(z; h) := \sup_{w \in X} \sup_{v \in X} \frac{dg(w, v; h)[z]}{\|w\|_X \|v\|_X}.$$

For **well-posedness** $\{u(\mu), \mu \in \mathcal{D}\}$ is required to be a **non-singular (isolated) branch**, thus we pose

Assumption

There is $\beta_0 > 0$, s.t. $\forall \mu \in \mathcal{D}: \beta(u(\mu); h(\mu)) \geq \beta_0$.

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Furthermore, we pose

Assumption

$\forall \mu \in \mathcal{D}$ there is $0 \leq \rho_a, \rho_b < \infty$, s.t. $\forall w, z, v \in X$:

$$\begin{aligned} |a(w, v; h_a)| &\leq \rho_a \|w\|_X \|v\|_X \|h_a\|_{L^\infty(\Omega)}, \\ |b(w, z, v; h_b)| &\leq \rho_b \|w\|_X \|z\|_X \|v\|_X \|h_b\|_{L^\infty(\Omega)}. \end{aligned}$$

In the sequel: $\rho_i(\mu) := \rho_i \|h_i(\mu)\|_{L^\infty(\Omega)}$, $i \in \{a, b\}$.

For $1 \leq N \leq N^{\max}$, let

- $S^N := \{\mu_n \in \mathcal{D}, 1 \leq n \leq N\}$ be a **nested set of parameter samples**, and
- $W^N := \text{span}\{\xi_n := u(\mu_n), 1 \leq n \leq N\}$ the associated **reduced-basis Lagrangian space**.

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Primal Reduced-Basis Problem:

$$\left\{ \begin{array}{l} \text{For } \mu \in \mathcal{D} \text{ find } \hat{u}(\mu) \in W^N, \text{ s.t. for all } v \in W^N: \\ g(\hat{u}(\mu), v; \hat{h}(\mu)) = 0, \end{array} \right.$$

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where we have replaced $h(\mu) := \{h_a(\mu), h_b(\mu)\}$ by $\hat{h}(\mu) := \{\hat{h}_a(\mu), \hat{h}_b(\mu)\}$ and

$$\hat{h}_i(\mu) := \sum_{m=1}^{M_i} \varphi_m^i(\mu) q_m^i, \quad i \in \{a, b\},$$

obtained by **Empirical Interpolation Method (EIM)**

(c.p. M. Barrault, Y. Maday, N.C. Nguyen, A.T. Patera; 2004).

Solved iteratively by **Newton's method**:

- Initial guess: $\hat{u}^{(0)}(\mu) \in W^N$.
- For $k = 0, 1, 2, \dots$:
 1. Find $\delta^{(k)}(\mu) \in W^N$, s.t. $\forall v \in W^N$:

$$dg(\delta^{(k)}(\mu), v; \hat{h}(\mu))[\hat{u}^{(k)}(\mu)] = -g(\hat{u}^{(k)}(\mu), v; \hat{h}(\mu));$$

2. Update $\hat{u}^{(k)}(\mu)$ by $\hat{u}^{(k+1)}(\mu) = \hat{u}^{(k)}(\mu) + \delta^{(k)}(\mu)$.

For the **offline/online decomposition**, let

$$\begin{aligned}
 \mathbf{F} &:= (f(\xi_i))_i, \\
 \mathbf{A}_m &:= (a(\xi_j, \xi_i; \mathbf{q}_m^a))_{i,j}, \quad 1 \leq m \leq M_a, \\
 \mathbf{B}_m^n &:= (b(\xi_j, \xi_n, \xi_i; \mathbf{q}_m^b))_{i,j}, \quad 1 \leq m \leq M_b, 1 \leq n \leq N, \\
 d\mathbf{B}_m^n &:= (db(\xi_j, \xi_i; \mathbf{q}_m^b) [\xi_n])_{i,j}, \quad 1 \leq m \leq M_b, 1 \leq n \leq N.
 \end{aligned}$$

The coefficients $\delta_n^{(k)}(\mu)$, $1 \leq n \leq N$, can be obtained by solving

$$\begin{aligned}
 &\left[\sum_{m=1}^{M_a} \varphi_m^a(\mu) \mathbf{A}_m + \sum_{n=1}^N \widehat{u}_n^{(k)}(\mu) \sum_{m=1}^{M_b} \varphi_m^b(\mu) d\mathbf{B}_m^n \right] \underline{\delta}^{(k)}(\mu) \\
 &= - \left[\sum_{m=1}^{M_a} \varphi_m^a(\mu) \mathbf{A}_m + \sum_{n=1}^N \widehat{u}_n^{(k)}(\mu) \sum_{m=1}^{M_b} \varphi_m^b(\mu) \mathbf{B}_m^n \right] \widehat{\underline{u}}^{(k)}(\mu) + \mathbf{F},
 \end{aligned}$$

within $\mathcal{O}(M_a N^2) + \mathcal{O}(M_b N^3) + \mathcal{O}(N^3)$.

\rightsquigarrow **(online-)complexity independent of $\mathcal{N} \gg N$.**

Improvement of the output approximation $\widehat{s}_1(\mu) := \ell(\widehat{u}(\mu))$ necessitates invoking the **Dual Problem**:

$$\left\{ \begin{array}{l} \text{For } \mu \in \mathcal{D} \text{ find } \psi(\mu) \in X, \text{ s.t. for all } v \in X: \\ dg\left(v, \psi(\mu); \widehat{u}(\mu) + \frac{1}{2}e(\mu); h(\mu)\right) = -\ell(v), \end{array} \right.$$

where $e(\mu) := u(\mu) - \widehat{u}(\mu)$.

\rightsquigarrow This is a **linear** problem.

For $1 \leq \tilde{N} \leq \tilde{N}^{\max}$, let

- $\tilde{\mathcal{S}}^{\tilde{N}} := \{\mu_n \in \mathcal{D}, 1 \leq n \leq \tilde{N}\}$ be a **nested set of parameter samples**, and
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Dual Reduced-Basis Problem:

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(Online-)complexity is $\mathcal{O}(M_a \tilde{N}^2) + \mathcal{O}(M_b N \tilde{N}^2) + \mathcal{O}(\tilde{N}^3)$.

\rightsquigarrow comparable to **one** Newton iteration (for solving the primal reduced-basis problem).

Existence, Uniqueness and Well-Posedness

First, we define a **proximity indicator** (the key parameter for the **BRR** theory):

$$\tau(\mu) := 4\rho_b(\mu)(\widehat{\beta}(\mu))^{-2}(R(\mu) + E(\mu)),$$

where (for $v \in X$ and $\mu \in \mathcal{D}$)

$$\begin{aligned} R(v; \mu) &:= g\left(\widehat{u}(\mu), v; \widehat{h}(\mu)\right), & R(\mu) &:= \|R(\cdot; \mu)\|_{X'}, \\ E(v; \mu) &:= g\left(\widehat{u}(\mu), v; h(\mu) - \widehat{h}(\mu)\right), & E(\mu) &:= \|E(\cdot; \mu)\|_{X'}, \end{aligned}$$

and $0 < \widehat{\beta}(\mu) \leq \beta(\widehat{u}(\mu); h(\mu))$ for all $\mu \in \mathcal{D}$.

Corollary

For $\tau(\mu) \leq \frac{1}{2}$ it is true, that $\beta(u(\mu); h(\mu)) \geq \widehat{\beta}(\mu)/\sqrt{2} > 0$.

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Immediate consequences:

- The primal problem is well-posed
($\{u(\mu), \mu \in \mathcal{D}\}$ is a non-singular (isolated) branch).
- The dual problem is well-posed and possesses a unique solution.

Proposition

For $\tau(\mu) < 1$ there is a unique $u(\mu)$ such that

- $u(\mu) \in \mathcal{B}(\hat{u}(\mu), \hat{\beta}(\mu) (2\rho_b(\mu))^{-1})$,
where $\mathcal{B}(z, r) := \{v \in X : \|v - z\|_X < r\}$,
- $\|u(\mu) - \hat{u}(\mu)\|_X \leq \Delta(\mu) := \hat{\beta}(\mu) (2\rho_b(\mu))^{-1} (1 - \sqrt{1 - \tau(\mu)})$.

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Proof: Use **Banach Fixed Point Theorem** for $H^\mu : X \rightarrow X$ defined by

$$dg(H^\mu w, v; h(\mu))[\hat{u}(\mu)] = dg(w, v; h(\mu))[\hat{u}(\mu)] - g(w, v; h(\mu)), \quad v \in X.$$

For the **dual problem** we define an **a-posteriori error estimator** by

$$\tilde{\Delta}(\mu) := \frac{2 \left(\tilde{R}(\mu) + \tilde{E}(\mu) \right)}{\hat{\beta}(\mu)(1 + \sqrt{1 - \tau(\mu)})} + \frac{(1 - \sqrt{1 - \tau(\mu)})}{(1 + \sqrt{1 - \tau(\mu)})} \left\| \hat{\psi}(\mu) \right\|_X,$$

where (similar to the primal problem)

$$\tilde{R}(\mu) := \left\| dg \left(\cdot, \hat{\psi}(\mu); \hat{u}(\mu); \hat{h}(\mu) \right) + \ell(\cdot) \right\|_{X'},$$

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We may proof that

Corollary

If $\tau(\mu) < 1$, then it holds $\left\| \psi(\mu) - \hat{\psi}(\mu) \right\|_X \leq \tilde{\Delta}(\mu)$.

For the **output of interest** we find $(\tilde{e}(\mu) := \psi(\mu) - \hat{\psi}(\mu))$:

$$s(\mu) - \underbrace{\ell(\hat{u}(\mu))}_{=: \hat{s}_1(\mu)} = R(\hat{\psi}(\mu); \mu) + E(\hat{\psi}(\mu); \mu) + g(\hat{u}(\mu), \tilde{e}(\mu); h(\mu)),$$

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or

$$s(\mu) - \underbrace{\left(\ell(\hat{u}(\mu)) + R(\hat{\psi}(\mu); \mu) \right)}_{=:\hat{s}_2(\mu)} = E(\hat{\psi}(\mu); \mu) + g(\hat{u}(\mu), \tilde{e}(\mu); h(\mu)).$$

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Therefore, for the corresponding **a-posteriori error estimators** we find

Corollary

If $\tau(\mu) < 1$, then it holds

1. $|s(\mu) - \hat{s}_1(\mu)| \leq \Delta_{s_1}(\mu) := \left| R(\hat{\psi}(\mu); \mu) \right| + \left| E(\hat{\psi}(\mu); \mu) \right| + (R(\mu) + E(\mu)) \tilde{\Delta}(\mu);$
2. $|s(\mu) - \hat{s}_2(\mu)| \leq \Delta_{s_2}(\mu) := \left| E(\hat{\psi}(\mu); \mu) \right| + (R(\mu) + E(\mu)) \tilde{\Delta}(\mu).$

Summary of quantities:

$$\tau(\mu): \quad R(\mu), E(\mu), \hat{\beta}(\mu),$$

$$\Delta(\mu): \quad \text{no additional terms,}$$

$$\tilde{\Delta}(\mu): \quad \tilde{R}(\mu), \tilde{E}(\mu), \left\| \hat{\psi}(\mu) \right\|_X,$$

$$\Delta_s(\mu): \quad R\left(\hat{\psi}(\mu); \mu\right), E\left(\hat{\psi}(\mu); \mu\right).$$

(Online-)complexity:

Summary of quantities:

$$\tau(\mu): \quad R(\mu), E(\mu), \hat{\beta}(\mu),$$

$$\Delta(\mu): \quad \text{no additional terms,}$$

$$\tilde{\Delta}(\mu): \quad \tilde{R}(\mu), \tilde{E}(\mu), \left\| \hat{\psi}(\mu) \right\|_{\mathcal{X}},$$

$$\Delta_s(\mu): \quad R\left(\hat{\psi}(\mu); \mu\right), E\left(\hat{\psi}(\mu); \mu\right).$$

(Online-)complexity:

$$R(\mu): \quad \mathcal{O}(M_b^2 N^4),$$

$$\tilde{R}(\mu): \quad \mathcal{O}(M_b^2 N^2 \tilde{N}^2),$$

Summary of quantities:

$$\tau(\mu): \quad R(\mu), E(\mu), \hat{\beta}(\mu),$$

$$\Delta(\mu): \quad \text{no additional terms,}$$

$$\tilde{\Delta}(\mu): \quad \tilde{R}(\mu), \tilde{E}(\mu), \|\hat{\psi}(\mu)\|_X,$$

$$\Delta_s(\mu): \quad R(\hat{\psi}(\mu); \mu), E(\hat{\psi}(\mu); \mu).$$

(Online-)complexity:

$$R(\mu): \quad \mathcal{O}(M_b^2 N^4), \quad E(\mu): \quad \mathcal{O}(N^4),$$

$$\tilde{R}(\mu): \quad \mathcal{O}(M_b^2 N^2 \tilde{N}^2), \quad \tilde{E}(\mu): \quad \mathcal{O}(N^2 \tilde{N}^2),$$

Summary of quantities:

$$\tau(\mu): \quad R(\mu), E(\mu), \hat{\beta}(\mu),$$

$$\Delta(\mu): \quad \text{no additional terms,}$$

$$\tilde{\Delta}(\mu): \quad \tilde{R}(\mu), \tilde{E}(\mu), \left\| \hat{\psi}(\mu) \right\|_X,$$

$$\Delta_s(\mu): \quad R(\hat{\psi}(\mu); \mu), E(\hat{\psi}(\mu); \mu).$$

(Online-)complexity:

$$R(\mu): \quad \mathcal{O}(M_b^2 N^4), \quad E(\mu): \quad \mathcal{O}(N^4),$$

$$\tilde{R}(\mu): \quad \mathcal{O}(M_b^2 N^2 \tilde{N}^2), \quad \tilde{E}(\mu): \quad \mathcal{O}(N^2 \tilde{N}^2),$$

$$R(\hat{\psi}(\mu); \mu): \quad \mathcal{O}(M_b N^2 \tilde{N}), \quad E(\hat{\psi}(\mu); \mu): \quad \mathcal{O}(N^2 \tilde{N}),$$

$$\left\| \hat{\psi}(\mu) \right\|_X: \quad \mathcal{O}(\tilde{N}^2).$$

Estimation of $\beta(\hat{u}(\mu), \hat{h}(\mu))$:

Let $\mathcal{F}(t; \bar{\mu})$ be an expansion of $(\beta(\hat{u}(\mu), \hat{h}(\mu)))^2$ in $\bar{\mu}$, s.t.

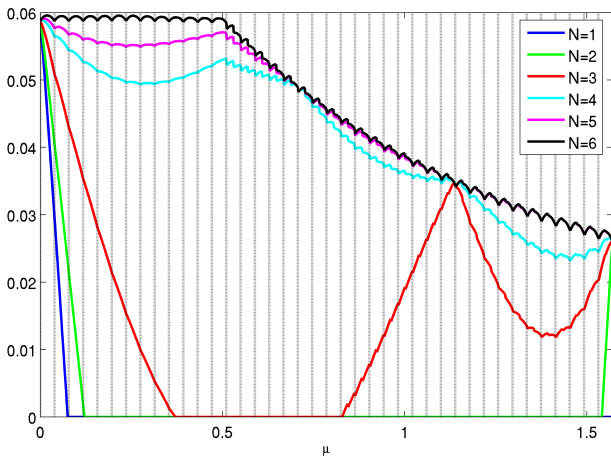
Corollary

1. $\mathcal{F}(t; \bar{\mu})$ is concave in t , i.e. $\forall t \in [t_1, t_2]: \mathcal{F}(t; \bar{\mu}) \geq \min\{\mathcal{F}(t_1; \bar{\mu}), \mathcal{F}(t_2; \bar{\mu})\}$.
2. For given $\mu, \bar{\mu} \in \mathcal{D}$, $t = \mu - \bar{\mu}$, the inf-sup parameter satisfies

$$\beta(\hat{u}(\mu); \hat{h}(\mu)) \geq \left(\sqrt{\mathcal{F}(t; \bar{\mu})} - \delta(t; \bar{\mu}) \right)^+,$$

where $\delta(t; \bar{\mu})$ is a **second order correction**.

Lower bound for **inf-sup** parameter:



Motivation

- Reduced-Basis Methods
- Application

Theory

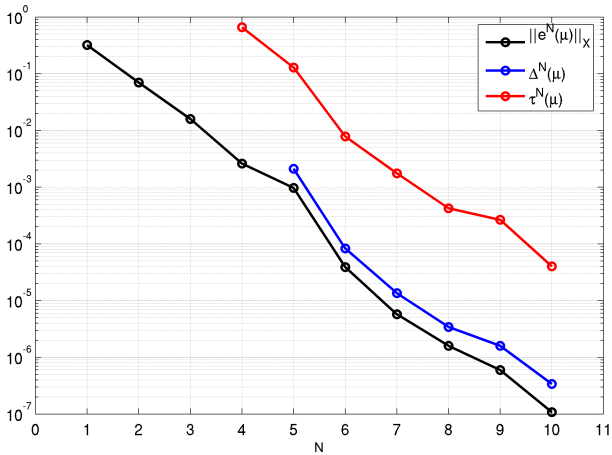
- Problem
 - Primal Problem
 - Dual Problem
 - Existence, Uniqueness and Well-Posedness
- A-Posteriori Error Estimation

Numerical Results

For $a = 0.1$, $\underline{b} = (0.5, 0.5)^T$ and $c = 0$ for the **Primal Problem** we obtain:

N	$\ e^N(\mu)\ _X$	$\Delta^N(\mu)$	$\eta^N(\mu)$	$\tau^N(\mu)$
2	7.02e-02	NaN	NaN	Inf
4	2.60e-03	NaN	NaN	6.61e-01
6	3.91e-05	8.32e-05	2.34e+00	7.85e-03
8	1.60e-06	3.43e-06	2.04e+00	4.25e-04
10	1.08e-07	3.40e-07	5.03e+00	4.02e-05

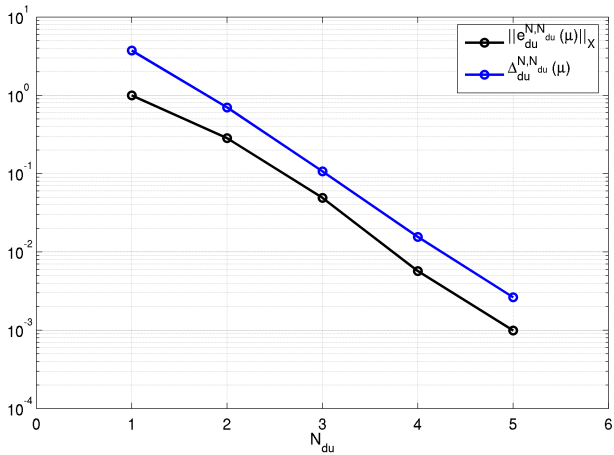
Where $e^N(\mu) := u(\mu) - \hat{u}^N(\mu)$ and $\eta^N(\mu) := \Delta^N(\mu) / \|e^N(\mu)\|_X$.



For the **Dual Problem** for fixed $N = N^{\max} = 10$:

\tilde{N}	$\ \tilde{e}^{N, \tilde{N}}(\mu)\ _X$	$\tilde{\Delta}^{N, \tilde{N}}(\mu)$	$\eta^{N, \tilde{N}}(\mu)$
1	9.99e-01	3.73e+00	3.03e+00
2	2.84e-01	7.00e-01	2.59e+00
3	4.91e-02	1.07e-01	2.52e+00
4	5.69e-03	1.56e-02	2.58e+00
5	9.91e-04	2.64e-03	4.06e+00

Where $\tilde{e}^{N, \tilde{N}}(\mu) := \psi^N(\mu) - \hat{\psi}^{N, \tilde{N}}(\mu)$ and $\hat{\eta}^{N, \tilde{N}}(\mu) := \tilde{\Delta}^{N, \tilde{N}}(\mu) / \|\tilde{e}^{N, \tilde{N}}(\mu)\|_X$.

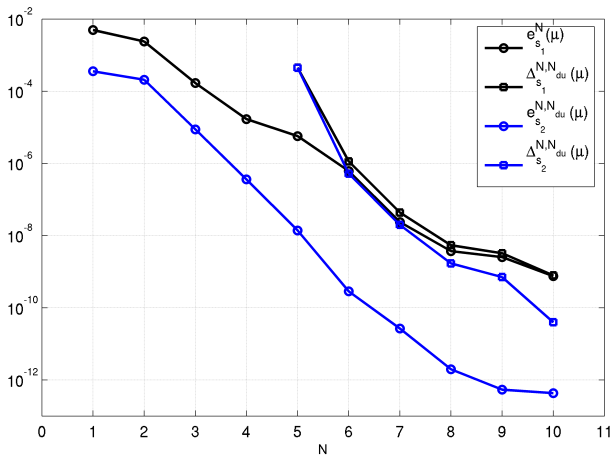


Output Approximation for $\tilde{N} = \tilde{N}^{\max} = 5$:

N	$e_{s_1}^N(\mu)$	$\Delta_{s_1}^{N, \tilde{N}}(\mu)$	$\eta_{s_1}^{N, \tilde{N}}(\mu)$	$e_{s_2}^{N, \tilde{N}}(\mu)$	$\Delta_{s_2}^{N, \tilde{N}}(\mu)$	$\eta_{s_2}^{N, \tilde{N}}(\mu)$
2	2.40e-03	NaN	NaN	2.08e-04	NaN	NaN
4	1.69e-05	NaN	NaN	3.60e-07	NaN	NaN
6	6.17e-07	1.14e-06	1.92e+00	2.86e-10	5.19e-07	2.45e+03
8	3.71e-09	5.40e-09	1.65e+00	1.97e-12	1.69e-09	8.56e+02
10	7.50e-10	7.89e-10	1.06e+00	4.33e-13	3.96e-11	1.66e+02

Where $e_{s_1}^N(\mu) := |s(\mu) - s_1^N(\mu)|$, $\eta_{s_1}^{N, \tilde{N}}(\mu) := \Delta_{s_1}^{N, \tilde{N}}(\mu)/e_{s_1}^N(\mu)$,

as well as, $e_{s_2}^{N, \tilde{N}}(\mu) := |s(\mu) - s_2^{N, \tilde{N}}(\mu)|$, $\eta_{s_2}^{N, \tilde{N}}(\mu) := \Delta_{s_2}^{N, \tilde{N}}(\mu)/e_{s_2}^{N, \tilde{N}}(\mu)$.



Computational savings (for the output approximation):

	$N = 2$	$N = 4$	$N = 6$	$N = 8$	$N = 10$
$\tilde{N} = 0$	385	364	346	328	311
$\tilde{N} = 1$	351	287	261	244	228
$\tilde{N} = 2$	349	285	258	240	224
$\tilde{N} = 3$	349	284	257	240	224
$\tilde{N} = 4$	349	284	257	240	223
$\tilde{N} = 5$	348	284	257	239	223

All computations are done with *Matlab 6.5* in conjunction with *Femlab 2.3* on an *AMD Opteron Processor 252* at 2.6 GHz

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