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Reduced Basis Methods for quadratically nonlinear PDEs with stochastic influences

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ECCOMAS 2012

Introduction

RB primal-dual formulation for linear outputs

RB dual formulations for quadratic outputs

Example

Problem Description

- $\mathcal{P} \subset \mathbb{R}^p$ set of deterministic parameters
- $(\Omega, \mathfrak{A}, \mathbb{P})$ probability space
- $D \subset \mathbb{R}^d$ open and bounded spatial domain
- $X \subset H^1(D)$ finite element space, $\dim(X) = \mathcal{N}$

Define parametrized stochastic forms

$a_0 : X \times X \times (\mathcal{P} \times \Omega) \to \mathbb{R}$	continuous bilinear form
$a_1 : X \times X \times X \times (\mathcal{P} \times \Omega) \to \mathbb{R}$	continuous trilinear form
$f : X \times (\mathcal{P} \times \Omega) \to \mathbb{R}$	bounded linear form

For $(\mu, \omega) \in \mathcal{P} \times \Omega$, we define

$$g(w, v; \mu, \omega) = a_0(w, v; \mu, \omega) + a_1(w, w, v; \mu, \omega) - f(v; \mu, \omega)$$

and the nonlinear, parametrized and random variational problem

find $u(\mu, \omega) \in X$ s.t. $\quad g(u(\mu, \omega), v; \mu, \omega) = 0, \quad \forall v \in X.$

Output of Interest

for a linear functional $\ell : X \times \mathcal{P} \to \mathbb{R}$

$$
\begin{aligned}
s(\mu,\omega) &:= \ell\left(u(\mu,\omega);\ \mu\right) \\
\mathbb{V}(\mu,\omega) &:= \mathbb{M}_2(\mu) - \mathbb{M}_1^2(\mu)
\end{aligned}
$$

where $\mathbb{M}_1(\mu)$ and $\mathbb{M}_2(\mu)$ denote first and second moment of $s(\mu,\cdot)$

Context

- weak solution in space
- strong solution in probability $\Rightarrow$ Monte Carlo evaluations

Motivation for Model Reduction

$\Rightarrow$ solutions for many parameters are required

$\Rightarrow$ solutions for many random realizations are required

Basic Idea of the RBM

Idea

- create reduced space $X_N \subset X$ "offline"
  - of dimension $N \ll \mathcal{N}$
  - made of snapshots, i.e. solutions for some pairs (μ, ω)
- solve problem on X_N "online"
  - find $u(\mu, \omega) \in X_N$ s.t. $g(u(\mu, \omega), v; \mu, \omega) = 0, \quad \forall v \in X_N$
  - complexity $\mathcal{O}(N^3)$ (for each Newton iteration)
- develop error bounds
  - confirm quality of the approximations of the reduced model
  - control size of reduced system

Requirements

- affine decomposition of g w.r.t. (μ, ω)
- i.e. separate x-dependent from (μ, ω)-dependent terms
  - to assemble system independent of $\mathcal{N}$
  - to evaluate error bounds independent of $\mathcal{N}$

Affine decomposition w.r.t. μ

Assumption: given by

$$g(w, v; \mu, \omega) = \sum_{q=1}^{Q} \theta_q(\mu) \cdot \left[\bar{g}_q(w, v) + g_q(w, v; \omega)\right]$$

- $\bar{g}_q$ represent the expectations
- g_q represent the fluctuating parts with zero mean

Affine decomposition w.r.t. ω

Karhunen-Loève (KL) Expansion

$$g_q(w, v; \omega) = \sum_{k=0}^{\bar{K}} \xi_{qk}(\omega)\, g_{qk}(w, v)$$

- random variables ξ_{qk} uncorrelated, zero mean, unit variance
- magnitude of g_{qk} typically decreases exponentially fast
- truncate at some $K \ll \bar{K} \Rightarrow$ truncated forms g_q^K, g^K, dg^K

Assembling a_0 "offline"

- Let $\{\varphi_1, ..., \varphi_{\mathcal{N}}\}$ be the (finite element) basis of X, assemble system matrix

$$a_0^K(\varphi_j, \varphi_i; \mu, \omega) = \sum_{q=1}^{Q} \sum_{k=0}^{K} \theta_q(\mu)\xi_{qk}(\omega)\ a_{0,qk}(\varphi_j, \varphi_i), \quad i, j = 1, ..., \mathcal{N}$$

- Let $\{\zeta_1, ..., \zeta_N\}$ be the (reduced) basis of X_N, $\quad \zeta_n = \sum_{i=1}^{\mathcal{N}} \zeta_{n,i}\varphi_i$, evaluate offline and store, independent of (μ, ω)

$$a_{0,qk}(\zeta_m, \zeta_n) = \sum_{i,j=1}^{\mathcal{N}} \zeta_{m,j}\zeta_{n,i}\ a_{0,qk}(\varphi_j, \varphi_i), \qquad n, m = 1, ..., N$$

Assembling a_0 "online"

- assemble online in $\mathcal{O}(QKN^2)$, independent of $\mathcal{N}$

$$a_0^K(\zeta_m, \zeta_n; \mu, \omega) = \sum_{q=1}^{Q} \sum_{k=0}^{K} \theta_q(\mu)\xi_{qk}(\omega)\ a_{0,qk}(\zeta_m, \zeta_n), \quad n, m = 1, ..., N$$

- similarly for a_1 in $\mathcal{O}(QKN^3)$ and f in $\mathcal{O}(QKN)$

Achievements

- reduced system independent of $\mathcal{N}$
  - assemble system in $\mathcal{O}(QKN^3)$
  - evaluate solution in $\mathcal{O}(N^3)$ per Newton step

Further Tasks

- develop error bounds
  - confirm quality of the approximations of the reduced model
  - selection of snapshots
  - control size of reduced system

primal-dual formulation: for $s(\mu,\omega)$ and $\mathbb{M}_1(\mu,\omega)$

Primal Formulations

- solutions $u_K \in X$ and $u_{NK} \in X_N$

$$\begin{aligned} g^K(u_K, v;\mu,\omega) &= 0, \qquad \forall v \in X,\\ g^K(u_{NK}, v;\mu,\omega) &= 0, \qquad \forall v \in X_N. \end{aligned}$$

Linear Dual Formulations

- solutions $p_K \in X$ and $p_{NK} \in \tilde{X}_N^p$

$$\begin{aligned} dg^K(v, p_K;\mu,\omega)[\tfrac{1}{2}(u+u_{NK})] &= -\ell(v;\mu), \qquad \forall v \in X,\\ dg^K(v, p_{NK};\mu,\omega)[u_{NK}] &= -\ell(v;\mu), \qquad \forall v \in \tilde{X}_N^p. \end{aligned}$$

- reduced space $\tilde{X}_N^p = \mathrm{span}(\{\zeta_n\}_{n=1}^{\tilde{N}^p}) \subset X, \quad \zeta_n := p_K(\mu_n,\omega_n)$
- Fréchet derivative

$$dg(w,v;\mu,\omega)[z] = a_0(w,v;\mu,\omega) + a_1(w,z,v;\mu,\omega) + a_1(z,w,v;\mu,\omega)$$

- complexity corresponds to one primal Newton iteration

solution error bounds

- Define the primal and dual **RB residual** as

$$
\begin{aligned}
r_{\mathrm{RB}}(v;\mu,\omega) &:= g^K(u_{NK}, v;\mu,\omega),\\
\tilde{r}^p_{\mathrm{RB}}(v;\mu,\omega) &:= dg^K(v, p_{NK})[u_{NK}] + \ell(v).
\end{aligned}
$$

- Define the primal and dual **KL "residual"** as

$$
\begin{aligned}
\delta_{\mathrm{KL}}(v;\mu,\omega) &:= \sum_{q=1}^{Q} \sum_{k=K+1}^{\bar{K}} \left|\theta_q(\mu)\,\xi_\varrho\, g_{qk}(u_{NK}, v)\right|,\\
\tilde{\delta}^p_{\mathrm{KL}}(v;\mu,\omega) &:= \sum_{q=1}^{Q} \sum_{k=K+1}^{\bar{K}} \left|\theta_q(\mu)\,\xi_\varrho\, dg_{qk}(v, p_{NK})[u_{NK}]\right|,
\end{aligned}
$$

where $|\xi_{qk}| \le \xi_\varrho$ holds with probability $1-\varrho$, $\quad 0 \le \varrho \ll 1$

solution error bounds

- Denote $\rho_1(\mu, \omega)$ the **continuity constant** of a_1
- Define the **inf-sup constant**

$$\beta(\mu, \omega) \;:=\; \inf_{w \in X} \sup_{v \in X} \frac{dg(w, v; \mu, \omega)[u_{NK}]}{\|w\|_X \|v\|_X}.$$

- Define the **RB and KL bounds**

$$\Delta_{\mathrm{RB}}(\mu, \omega) := \frac{1}{\beta_{\mathrm{LB}}} \sup_{v \in X} \left(\frac{r_{\mathrm{RB}}(v)}{\|v\|_X} \right), \quad \tilde{\Delta}^p_{\mathrm{RB}}(\mu, \omega) := \frac{1}{\beta_{\mathrm{LB}}} \sup_{v \in X} \left(\frac{\tilde{r}^p_{\mathrm{RB}}(v)}{\|v\|_X} \right),$$

$$\Delta_{\mathrm{KL}}(\mu, \omega) := \frac{1}{\beta_{\mathrm{LB}}} \sup_{v \in X} \left(\frac{\delta_{\mathrm{KL}}(v)}{\|v\|_X} \right), \quad \tilde{\Delta}^p_{\mathrm{KL}}(\mu, \omega) := \frac{1}{\beta_{\mathrm{LB}}} \sup_{v \in X} \left(\frac{\tilde{\delta}^p_{\mathrm{KL}}(v)}{\|v\|_X} \right).$$

  - use Riesz representators of affine terms for evaluation
  - online complexity $\mathcal{O}(Q^2 \bar{K}^2 N^4)$ independent of $\mathcal{N}$

solution error bounds

For $2(\Delta_{\mathrm{RB}}+\Delta_{\mathrm{KL}}) < \frac{\beta_{\mathrm{LB}}}{2\rho_1}$, we define the bounds

$$
\begin{aligned}
\Delta(\mu,\omega) &:= 2\big(\Delta_{\mathrm{RB}} + \Delta_{\mathrm{KL}}\big) \\
\tilde{\Delta}^p(\mu,\omega) &:= 2\big(\tilde{\Delta}^p_{\mathrm{RB}} + \tilde{\Delta}^p_{\mathrm{KL}}\big) + \frac{2\rho_1}{\beta_{\mathrm{LB}}}\Delta\|p_{NK}\|_X
\end{aligned}
$$

such that there exists a unique solution $u(\mu,\omega) \in B\big(u_{NK}, \frac{\beta_{\mathrm{LB}}}{2\rho_1}\big)$ and

$$
\begin{aligned}
\|u(\mu,\omega) - u_{NK}(\mu,\omega)\|_X &\leq \Delta(\mu,\omega) \\
\|p(\mu,\omega) - p_{NK}(\mu,\omega)\|_X &\leq \tilde{\Delta}^p(\mu,\omega)
\end{aligned}
$$

Proof: based upon Brezzi-Rappaz-Raviart theory

output error bounds

Linear Output Approximation

$$s_{NK}(\mu,\omega) := \ell(u_{NK}) + r_{\mathrm{RB}}(p_{NK})$$
$$\mathbb{M}_{1,NK}(\mu) := \mathbb{E}[s_{NK}(\mu,\cdot)]$$

- $s_{NK} \neq \ell(u_{NK})$
- $r_{\mathrm{RB}}(p_{NK})$ added as "correction" term

Linear Output Bounds

$$\Delta^s(\mu,\omega) := \beta_{\mathrm{LB}}\Delta\tilde{\Delta}^p + \delta_{\mathrm{KL}}(p_{NK})$$
$$\Delta^{\mathbb{M}_1}(\mu) := \mathbb{E}\left[\Delta^s(\mu,\cdot)\right]$$

- Δ_{RB}, Δ_{KL} appear in products with each other

$\Rightarrow$ only small N and K necessary

- δ_{KL} is more precise than Δ_{KL} and decreases fast in K

additional dual formulation: for $s^2(\mu,\omega)$ and $\mathbb{M}_1^2(\mu,\omega)$

Additional Linear Dual Formulations

- Analogously to the first dual problem:
- solutions $y_K \in X$ and $y_{NK} \in \tilde{X}_N^y$
  solutions $z_K \in X$ and $z_{NK} \in \tilde{X}_N^z$

$$
\begin{aligned}
dg^K(v, y_K; \mu,\omega)[\tfrac{1}{2}(u+u_{NK})] &= -2s_{NK}(\mu,\omega)\,\ell(v;\mu), \quad \forall v \in X,\\
dg^K(v, z_K; \mu,\omega)[\tfrac{1}{2}(u+u_{NK})] &= -2\mathbb{M}_{1,NK}(\mu,\omega)\,\ell(v;\mu), \ \forall v \in X.
\end{aligned}
$$

$$
\begin{aligned}
dg^K(v, y_{NK}; \mu,\omega)[u_{NK}] &= -2s_{NK}(\mu,\omega)\,\ell(v;\mu), \quad \forall v \in \tilde{X}_N^y,\\
dg^K(v, z_{NK}; \mu,\omega)[u_{NK}] &= -2\mathbb{M}_{1,NK}(\mu,\omega)\,\ell(v;\mu), \ \forall v \in \tilde{X}_N^z.
\end{aligned}
$$

- in practice, we use $\tilde{X}_N^z = \tilde{X}_N^y$

quadratic outputs

Quadratic Output Approximation

$$
\begin{aligned}
s_{NK}^{[2]}(\mu,\omega) &:= (s_{NK})^2 \quad + \quad 2\, s_{NK} \quad r_{\mathrm{RB}}(p_{NK}) - r_{\mathrm{RB}}(y_{NK})\,, \\
\mathbb{M}_{1,NK}^{[2]}(\mu) &:= (\mathbb{M}_{1,NK})^2 + \mathbb{E}\left[2\mathbb{M}_{1,NK} r_{\mathrm{RB}}(p_{NK}) - r_{\mathrm{RB}}(z_{NK})\right],
\end{aligned}
$$

- Additional “correction” terms
- Alternatively: $s_{NK}^{[2]} := \ell^2(u^{NK}) - r_{\mathrm{RB}}^2(p_{NK}) - r_{\mathrm{RB}}(y_{NK})$

Second Moment and Variance

$$
\mathbb{V}_{NK}(\mu) := \mathbb{E}\left[s_{NK}^{[2]}(\mu,\cdot)\right] - \mathbb{M}_{1,NK}^{[2]}(\mu)
$$

quadratic output error bounds

LINEAR OUTPUT BOUNDS: $\Delta^s(\mu,\omega) := \beta_{LB}\Delta\tilde{\Delta}^p + \delta_{KL}(p_{NK})$

QUADRATIC OUTPUT BOUNDS

$$\begin{aligned} \Delta^{s^2}(\mu,\omega) &:= (\Delta^s)^2 + \beta_{LB}\Delta\tilde{\Delta}^y + \delta_{KL}(y_{NK}), \\ \Delta^{\mathbb{M}_1^2}(\mu) &:= (\Delta^{\mathbb{M}_1})^2 + \mathbb{E}\left[\beta_{LB}\Delta\tilde{\Delta}^z + \delta_{KL}(z_{NK})\right]. \end{aligned}$$

- Δ^s is already small $\Rightarrow (\Delta^s)^2$ almost negligible

$\Rightarrow$ Δ^{s^2} will probably be of the same order than Δ^s

VARIANCE OUTPUT BOUNDS

$$\begin{aligned} \Delta^{\mathbb{V}}(\mu) := \; & \mathbb{E}\left[(\Delta^s)^2\right] + (\Delta^{\mathbb{M}_1})^2 \\ & + \mathbb{E}\left[\beta_{LB}\Delta\tilde{\Delta}^{y-z} + \delta_{KL}(y_{NK} - z_{NK})\right] \end{aligned}$$

Achievements

- reduced system
  - assemble system in $\mathcal{O}(QKN^3)$
  - evaluate solution in $\mathcal{O}(N^3)$ per Newton step
- efficient dual problems
  - complexity corresponds to one primal Newton iteration
- error bounds
  - for s, s^2, $\mathbb{M}_1$, $\mathbb{M}_2$ and $\mathbb{V}$
  - all bounds are likely to be of the same order
  - computational complexity $\mathcal{O}(Q^2\bar{K}^2N^4)$
  - we can derive sharper error bounds (see paper)

EXAMPLE: stationary convection-diffusion process

CONCENTRATION/MASS TRANSPORT IN A WET SANDSTONE

parameter and constants

- $\mu_1 \in [0.05, 1.00]$ global water saturation in the pores
- $\mu_2 \in [0.20, 1.00]$ convection magnitude
- $\kappa : D \times \Omega \to [0, 1]$ rate of pore space per control volume
- diffusivities: $\eta_s = 0.04$ of sandstone, $\eta_w = 3.10$ of water, $\eta_a = 1.20$ of air

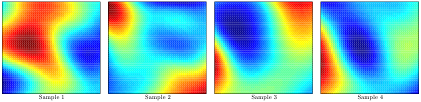
coefficients

- $\eta(\mu, \omega)$ diffusivity, depending on η_s, η_w, η_a, $\kappa(\omega)$ and μ_1
- $\vec{\nu}(\mu_2)$ convection, depending on μ_2
- $\gamma(\omega)$ random zero mean Neumann outlet condition

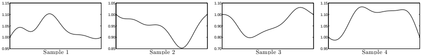
$$\begin{cases} -\nabla \cdot \big(\eta(\mu,\omega)\, \nabla u(\mu,\omega)\big) + \vec{\nu}(\mu_2) \cdot \nabla u\, u & = & 0 \quad \text{in } D, \\ \quad u(\mu,\omega) & = & 0 \quad \text{on } \Gamma_D, \\ \quad n \cdot \big(\eta(\mu_1,\omega)\, \nabla u(\mu,\omega)\big) & = & 0 \quad \text{on } \Gamma_N, \\ \quad n \cdot \big(\eta(\mu_1,\omega)\, \nabla u(\mu,\omega)\big) & = & \gamma(\omega) \quad \text{on } \Gamma_{out}. \end{cases}$$

eigenvalues and truncation values of the KL expansions

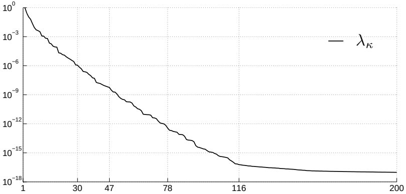
Four random realizations of κ



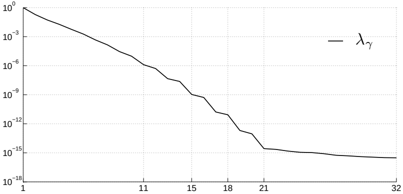
Four random realizations of γ



KL Eigenvalues of κ



KL Eigenvalues of γ



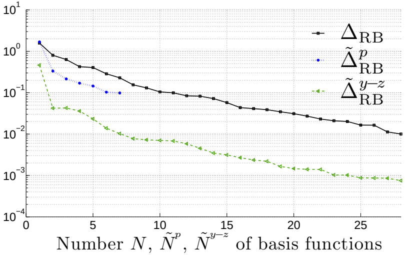
KL truncation values

- $K_\kappa = 30$
- $\bar{K}_\kappa = 47$

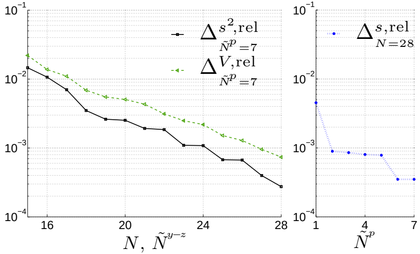
KL truncation values

- $K_\gamma = 11$
- $\bar{K}_\gamma = 15$

Error Decay



(a) RB error decay of primal solution u and dual solutions p and $(y-z)$



(b) rel. error decay of outputs s, s^2 and $\mathbb{V}$ without δ_{KL}-contributions

Results

For error tolerance 10^{-3}

- needed basis functions
- speedup factor:
  full system to reduced system

$\mathcal{N}$	$(N, \tilde{N}^p, \tilde{N}^y)$	speedup
3.191	(28, 7, 28)	33
12.555	(28, 7, 28)	96

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