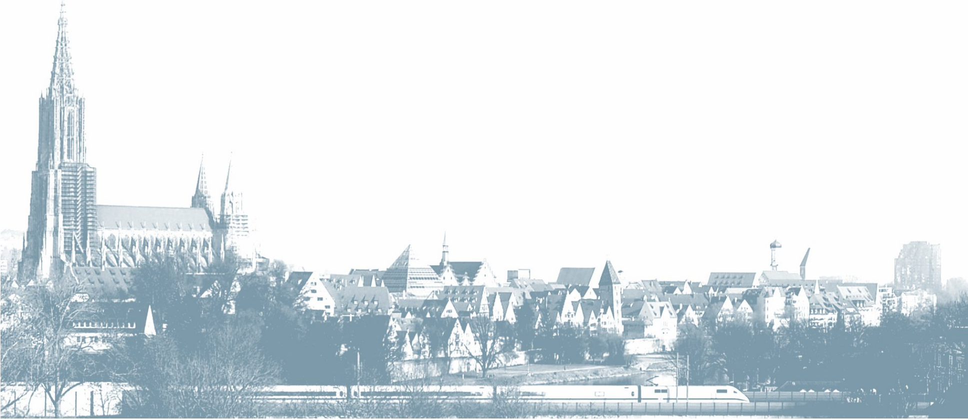

Reduced Basis Methods for parametrized PDEs with stochastic influences

Bernhard Wieland | January 22, 2013 | Leipzig
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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[1] forms

$a : X \times X \times (\mathcal{P} \times \Omega) \to \mathbb{R}$ continuous bilinear form

$f : X \times \mathcal{P} \to \mathbb{R}$ bounded linear form

For $(\mu, \omega) \in \mathcal{P} \times \Omega$, we define the linear, parametrized, and random variational problem:

Find $u(\mu, \omega) \in X$ s.t.

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

[1] $f : X \times (\mathcal{P} \times \Omega) \to \mathbb{R}$ possible. Assumed to be deterministic only for notational reasons.

Output of Interest

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

$$s(\mu,\omega) := \ell\,(u(\mu,\omega);\ \mu)$$
$$\mathbb{V}(\mu,\omega) := \mathbb{M}_2(\mu) - \mathbb{M}_1^2(\mu)$$

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.

$$a(u(\mu, \omega), v; \mu, \omega) = f(v; \mu), \quad \forall v \in X_N.$$

  - run-time complexity $\mathcal{O}(N^3)$ for each $(\mu, \omega) \in \mathcal{P} \times \Omega$
- develop error bounds
  - confirm quality of the approximations of the reduced model
  - control size of reduced system

Requirements

- affine decomposition of a, f, and ℓ 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

$$f(v;\mu) = \sum_{q=1}^{Q^f} \theta_q^f(\mu) \cdot f_q(v), \qquad \ell(v;\mu) = \sum_{q=1}^{Q^\ell} \theta_q^\ell(\mu) \cdot \ell_q(v)$$

$$a(w,v;\mu,\omega) = \sum_{q=1}^{Q^a} \theta_q^a(\mu) \cdot a_q(w,v;\omega)$$

Affine decomposition of a_q w.r.t. ω

Karhunen-Loève (KL) Expansion

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

- $\xi_{q0} = 1$ and a_{q0} represents the mean of a_q
- random variables ξ_{qk} uncorrelated, zero mean, unit variance
- magnitude of a_{qk} decreases, typically exponentially fast
- truncate at some $K \ll \bar{K} \Rightarrow$ truncated forms a_q^K, a^K

"Offline" assembling of a

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

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

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

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

- storage complexity[2] $\mathcal{O}(QKN^2)$

"Offline" assembling of f and ℓ

- analogously store $f_q(\zeta_n)$ and $\ell_q(\zeta_n)$
- storage complexities[2] for f and ℓ are $\mathcal{O}(QN)$

[2] For notational simplicity we use $Q = Q^a = Q^f = Q^\ell$

"Online" assembling of a

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

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

"Online" assembling of f and ℓ

- analogously for f and ℓ in $\mathcal{O}(QN)$

$$f(\zeta_n; \mu) = \sum_{q=1}^{Q} \theta_q^f(\mu)\; f_q(\zeta_n), \quad n = 1, ..., N$$

$$\ell(\zeta_n; \mu) = \sum_{q=1}^{Q} \theta_q^\ell(\mu)\; \ell_q(\zeta_n), \quad n = 1, ..., N$$

Achievements

- reduced system independent of $\mathcal{N}$
  - assemble system in $\mathcal{O}(QKN^2)$
  - evaluate solution in $\mathcal{O}(N^3)$

Further Tasks

- develop error bounds
  - confirm quality of approximations of 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 $u_{N,K} \in X_N$

$$\begin{aligned} a^K(u_K, v; \mu, \omega) &= f(v; \mu), \qquad \forall v \in X \\ a^K(u_{N,K}, v; \mu, \omega) &= f(v; \mu), \qquad \forall v \in X_N \end{aligned}$$

LINEAR DUAL FORMULATIONS

- solutions $p_K^{(1)} \in X$ and $p_{N,K}^{(1)} \in \tilde{X}_N^{(1)}$

$$\begin{aligned} a^K(v, p_K^{(1)}; \mu, \omega) &= -\ell(v; \mu), \qquad \forall v \in X \\ a^K(v, p_{N,K}^{(1)}; \mu, \omega) &= -\ell(v; \mu), \qquad \forall v \in \tilde{X}_N^{(1)} \end{aligned}$$

- reduced space $\tilde{X}_N^{(1)} = \mathrm{span}(\{\zeta_n\}_{n=1}^{\tilde{N}^{(1)}}) \subset X, \quad \zeta_n := p_K^{(1)}(\mu_n, \omega_n)$
- complexity corresponds to one primal solution

solution error bounds

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

$$r_{\mathrm{RB}}(v;\mu,\omega) := f(v;\mu) - a^K(u_{N,K}(\mu,\omega), v;\,\mu,\omega), \quad v \in X$$
$$\tilde{r}^{(1)}_{\mathrm{RB}}(v;\mu,\omega) := \ell(v;\mu) + a^K(v, p^{(1)}_{N,K}(\mu,\omega);\,\mu,\omega), \quad v \in X$$

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

$$\delta_{\mathrm{KL}}(v;\mu,\omega) := \sum_{q=1}^{Q} \sum_{k=K+1}^{\bar{K}} \left|\theta^a_q(\mu)\,\xi_\varrho\, a_{qk}(u_{N,K}(\mu,\omega), v)\right|, \quad v \in X$$
$$\tilde{\delta}^{(1)}_{\mathrm{KL}}(v;\mu,\omega) := \sum_{q=1}^{Q} \sum_{k=K+1}^{\bar{K}} \left|\theta^a_q(\mu)\,\xi_\varrho\, a_{qk}(v, p^{(1)}_{N,K}(\mu,\omega))\right|, \quad v \in X$$

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

solution error bounds

- Define the **coercivity constant**

$$\alpha(\mu,\omega) \;:=\; \inf_{v\in X} \frac{a(v,v;\mu,\omega)}{\|v\|_X^2} \;\geq\; \alpha_0 \;>\; 0$$

- Define the **RB and KL bounds**

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

$$\Delta_{KL}(\mu,\omega) := \frac{1}{\alpha_{LB}} \sup_{v\in X}\left(\frac{\delta_{KL}(v)}{\|v\|_X}\right) \qquad \tilde{\Delta}^{(1)}_{KL}(\mu,\omega) := \frac{1}{\alpha_{LB}} \sup_{v\in X}\left(\frac{\tilde{\delta}^{(1)}_{KL}(v)}{\|v\|_X}\right)$$

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

-

$$\begin{aligned}
\|u(\mu,\omega) - u_{N,K}(\mu,\omega)\|_X &\leq \Delta(\mu,\omega) &&:= \Delta_{RB} + \Delta_{KL} \\
\|p^{(1)}(\mu,\omega) - p^{(1)}_{N,K}(\mu,\omega)\|_X &\leq \tilde{\Delta}^{(1)}(\mu,\omega) &&:= \tilde{\Delta}^{(1)}_{RB} + \tilde{\Delta}^{(1)}_{KL}
\end{aligned}$$

output error bounds

Linear Output Approximation

$$
\begin{aligned}
s_{N,K}(\mu,\omega) &:= \ell(u_{N,K}) - r_{\mathrm{RB}}(p^{(1)}_{N,K}) \\
\mathbb{M}_{1,NK}(\mu) &:= \mathbb{E}[s_{N,K}(\mu,\cdot)]
\end{aligned}
$$

- $s_{N,K} \neq \ell(u_{N,K})$
- $r_{\mathrm{RB}}(p^{(1)}_{N,K})$ added as “correction” term

Linear Output Bounds

$$
\begin{aligned}
|s - s_{N,K}| &\leq \Delta^s(\mu,\omega) := \alpha_{\mathrm{LB}}\Delta\tilde{\Delta}^{(1)} + \delta_{\mathrm{KL}}(p^{(1)}_{N,K}) \\
|\mathbb{M}_1 - \mathbb{M}_{1,NK}| &\leq \Delta^{\mathbb{M}_1}(\mu) := \mathbb{E}\left[\alpha_{\mathrm{LB}}\Delta\tilde{\Delta}^{(1)}\right]
\end{aligned}
$$

- 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

Outline of the Proof

$$|s - s_{N,K}| \quad \leq \quad \Delta^s \quad = \quad \alpha_{\mathrm{LB}} \Delta \tilde{\Delta}^{(1)} \; + \; \delta_{\mathrm{KL}}(p_{N,K}^{(1)})$$

$$\begin{aligned} s - s_{N,K} &= \ell(u) - \ell(u_{N,K}) + r_{\mathrm{RB}}(p_{N,K}^{(1)}) \\ &= -a^K(e, p_K^{(1)}) \quad + r_{\mathrm{RB}}(p_{N,K}^{(1)}) \qquad\qquad \text{where } \; e = u - u_{N,K} \\ &= -a^K(e, p_K^{(1)}) \quad + a(u, p_{N,K}^{(1)}) - a^K(u_{N,K}, p_{N,K}^{(1)}) \\ &= \tilde{r}_{\mathrm{RB}}^{(1)}(e) \; + \; [a - a^K](u, p_{N,K}^{(1)}) \\ &= \underbrace{\tilde{r}_{\mathrm{RB}}^{(1)}(e)}_{\leq \alpha_{\mathrm{LB}} \, \Delta \, \tilde{\Delta}_{\mathrm{RB}}^{(1)}} \; + \; \underbrace{[a - a^K](e, p_{N,K}^{(1)})}_{\leq \alpha_{\mathrm{LB}} \, \Delta \, \tilde{\Delta}_{\mathrm{KL}}^{(1)}} \; + \; \underbrace{[a - a^K](u_{N,K}, p_{N,K}^{(1)})}_{\leq \delta_{\mathrm{KL}}(p_{N,K}^{(1)})} \end{aligned}$$

$$|\mathbb{M}_1 - \mathbb{M}_{1,NK}| \quad \leq \quad \Delta^{\mathbb{M}_1} \quad = \quad \mathbb{E}\left[\alpha_{\mathrm{LB}} \Delta \tilde{\Delta}^{(1)}\right]$$

Since $\{\xi_{q,k}, \; k > K\}$ and $\{\xi_{q,k}, \; k \leq K\}$ uncorrelated and $\mathbb{E}[\xi_{qk}] = 0$, we have

$$\mathbb{E}\left[[a - a^K](u_{N,K}, p_{N,K}^{(1)}) \right] = \sum_{q=1}^{Q} \sum_{k>K} \theta_q^a(\mu) \, \mathbb{E}[\xi_{qk}] \cdot \mathbb{E}[\underbrace{a_{qk}(u_{N,K}, p_{N,K}^{(1)})}_{\text{depends on } \xi_{q,k},\, k \leq K}] \; = \; 0$$

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 $p_K^{(2)} \in X$ and $p_{N,K}^{(2)} \in \tilde{X}_N^{(2)}$
  solutions $p_K^{(3)} \in X$ and $p_{N,K}^{(3)} \in \tilde{X}_N^{(3)}$

$$
\begin{aligned}
a^K(v, p_K^{(2)}; \mu, \omega) &= -2 s_{N,K}(\mu,\omega)\, \ell(v;\mu), \quad \forall v \in X \\
a^K(v, p_K^{(3)}; \mu, \omega) &= -2 \mathbb{M}_{1,NK}(\mu,\omega)\, \ell(v;\mu), \; \forall v \in X
\end{aligned}
$$

$$
\begin{aligned}
a^K(v, p_{N,K}^{(2)}; \mu, \omega) &= -2 s_{N,K}(\mu,\omega)\, \ell(v;\mu), \quad \forall v \in \tilde{X}_N^{(2)} \\
a^K(v, p_{N,K}^{(3)}; \mu, \omega) &= -2 \mathbb{M}_{1,NK}(\mu,\omega)\, \ell(v;\mu), \; \forall v \in \tilde{X}_N^{(3)}
\end{aligned}
$$

- in practice, we use $\tilde{X}_N^{(3)} = \tilde{X}_N^{(2)}$

quadratic outputs

Quadratic Output Approximation

$$s^{[2]}_{N,K}(\mu,\omega) := (s_{N,K})^2 + 2\, s_{N,K}\; r_{\mathrm{RB}}(p^{(1)}_{N,K}) - r_{\mathrm{RB}}(p^{(2)}_{N,K})$$
$$\mathbb{M}^{[2]}_{1,NK}(\mu) := (\mathbb{M}_{1,NK})^2 + \mathbb{E}\left[2\mathbb{M}_{1,NK}\, r_{\mathrm{RB}}(p^{(1)}_{N,K}) - r_{\mathrm{RB}}(p^{(3)}_{N,K})\right]$$

- Additional “correction” terms
- Alternatively: $s^{[2]}_{N,K} := \ell^2(u_{N,K}) - r^2_{\mathrm{RB}}(p^{(1)}_{N,K}) - r_{\mathrm{RB}}(p^{(2)}_{N,K})$

Second Moment and Variance

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

quadratic output error bounds

$$\Rightarrow \quad s^2 - s^{[2]}_{N,K} = s^2 - (s_{N,K})^2 - 2 s_{N,K} r_{\text{RB}}(p^{(1)}_{N,K}) + r_{\text{RB}}(p^{(2)}_{N,K})$$

Consider the first part:

$$s^2 - (s_{N,K})^2 = (s - s_{N,K})^2 + 2 s_{N,K} (s - s_{N,K})$$

Furthermore

$$\begin{aligned} 2 s_{N,K} (s - s_{N,K}) &= 2 s_{N,K} \ell(u) - 2 s_{N,K} \ell(u_{N,K}) + 2 s_{N,K} r_{\text{RB}}(p^{(1)}_{N,K}) \\ &= -a^K(e, p^{(2)}_K) \qquad\qquad + 2 s_{N,K} r_{\text{RB}}(p^{(1)}_{N,K}) \end{aligned}$$

$$\Rightarrow \quad s^2 - s^{[2]}_{N,K} = \underbrace{(s - s_{N,K})^2}_{\leq (\Delta^s)^2} \quad \underbrace{- a^K(e, p^{(2)}_K) + r_{\text{RB}}(p^{(2)}_{N,K})}_{\text{linear: } s - s_{N,K} = -a^K(e, p^{(1)}_K) + r_{\text{RB}}(p^{(1)}_{N,K})}$$

quadratic output error bounds

LINEAR OUTPUT BOUNDS: $\Delta^s(\mu,\omega) := \alpha_{\mathrm{LB}} \Delta\tilde{\Delta}^{(1)} + \delta_{\mathrm{KL}}(p_{N,K}^{(1)})$

QUADRATIC OUTPUT BOUNDS

$$\Delta^{s^2}(\mu,\omega) := (\Delta^s)^2 + \alpha_{\mathrm{LB}} \Delta\tilde{\Delta}^{(2)} + \delta_{\mathrm{KL}}(p_{N,K}^{(2)})$$

$$\Delta^{\mathbb{M}_1^2}(\mu) := (\Delta^{\mathbb{M}_1})^2 + \mathbb{E}\left[\alpha_{\mathrm{LB}} \Delta\tilde{\Delta}^{(3)}\right]$$

- 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

$$\Delta^{\mathbb{V}}(\mu) := \mathbb{E}\left[(\Delta^s)^2\right] + (\Delta^{\mathbb{M}_1})^2 + \mathbb{E}\left[\alpha_{\mathrm{LB}} \Delta\tilde{\Delta}^{(2-3)}\right]$$

Achievements

- reduced system
  - assemble system in $\mathcal{O}(QKN^2)$
  - evaluate solution in $\mathcal{O}(N^3)$
- efficient dual problems
  - complexity corresponds to one primal solution
  - (in nonlinear setting to one 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 $\mathcal{O}(Q^2\bar{K}^2N^2)$

EXAMPLE: two-dimensional porous medium

HEAT TRANSFER IN A WET SANDSTONE

parameter and constants

- $\mu \in [0.01, 1.00]$ global water saturation in the pores
- $\kappa : D \times \Omega \rightarrow [0, 1]$ rate of pore space per control volume
- heat conductivities: *sandstone* : $\eta_s = 2.40$, water: $\eta_w = 0.60$, air: $\eta_a = 0.03$

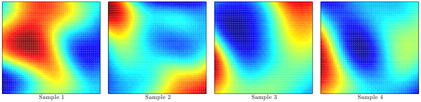
coefficients

- $c(\mu, \omega)$ conductivity, depending on η_s, η_w, η_a, $\kappa(\omega)$ and μ
- $\gamma(\omega)$ random zero mean Neumann outlet condition

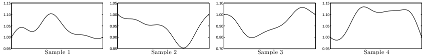
$$\begin{cases} -\nabla \cdot \Big(c(\mu,\omega)\, \nabla u(\mu,\omega) \Big) & = & 0 & \text{in } D \\ u(\mu,\omega) & = & 0 & \text{on } \Gamma_D \\ \vec{n} \cdot \Big(c(\mu,\omega)\, \nabla u(\mu,\omega) \Big) & = & 0 & \text{on } \Gamma_N \\ \vec{n} \cdot \Big(c(\mu,\omega)\, \nabla u(\mu,\omega) \Big) & = & \gamma(\omega) & \text{on } \Gamma_{\text{out}} \end{cases}$$

eigenvalues and truncation values of the KL expansions

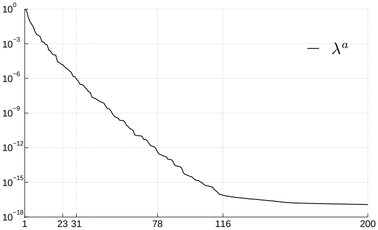
Four random realizations of κ



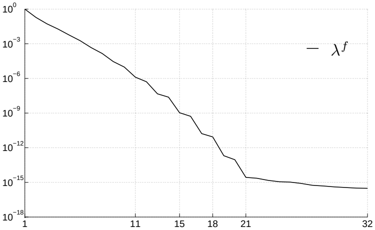
Four random realizations of γ



KL Eigenvalues of κ



KL Eigenvalues of γ



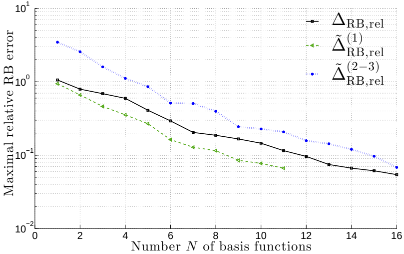
KL truncation values

- $K_\kappa = 23$
- $\bar{K}_\kappa = 31$

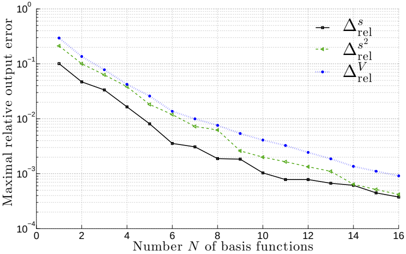
KL truncation values

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

Error Decay



(a) RB error decay of primal solution u and dual solutions $p^{(1)}$ and $(p^{(2)} - p^{(3)})$



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

Results

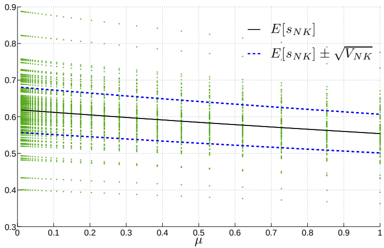
For error tolerance 10^{-3}

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

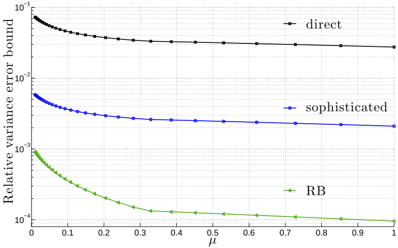
$\mathcal{N}$	$(N, \tilde{N}^{(1)}, \tilde{N}^{(2)})$	speedup
4.841	$(16, 11, 16)$	35
19.121	$(16, 11, 16)$	138

Results

For a test set of 30 logarithmically distributed values of μ



(c) First moment $\mathbb{M}_1(\mu)$, standard deviation $\sigma(\mu) = \sqrt{\mathbb{V}(\mu)}$ and 100 random samples



(d) relative error bounds for variance $\mathbb{V}(\mu)$:
– sophisticated is ∼12 times larger in average
– direct is ∼160 times larger in average

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