

Reduced Basis Approach for PDEs with Stochastic Parameters: Heat Conduction with Variable Robin Coefficient

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Outline of the talk

Reduced-Basis for PDEs with Stochastic Parameters : Overview

Motivation – Model Problem

Computation Strategy

Technical Details

Assumptions on the Random Input Field B_i

RB for BVP with Deterministic Parameters

Numerical results

Reduced-Basis (RB) [1] (=model reduction) approach for Boundary Value Problems (BVP) with **stochastic parameters** $\mu(\omega)$:

- ▶ Partial Differential Equation (PDE: operator A , functions U, f)

$$A(\mu(\omega)) U(\mu(\omega)) = f(\mu(\omega)) \text{ in } \mathcal{D} ,$$

- ▶ Boundary Condition (BC: operator B , trace of U , function g)

$$B(\mu(\omega)) U(\mu(\omega)) = g(\mu(\omega)) \text{ in } \partial\mathcal{D} .$$

- ▶ **Multiscale** model [2]: **macro** U influenced by **micro** $\mu(\omega)$.

[1] C. Prud'homme, D. Rovas, K. Veroy, Y. Maday, A.T. Patera, and G. Turinici. Reliable real-time solution of parametrized partial differential equations: Reduced-basis output bounds methods. JFE, 124(1):7–80, 2002.

[2] S. Boyaval. Reduced-basis approach for homogenization beyond the periodic setting. SIAM MMS, 7(1):466–494, 2008.

Model Problem with Stochastic Parameters

Laplace equation for $U(x, \omega) \in H^1(\mathcal{D})$, \forall a.e. $\omega \in (\Omega, \mathcal{F}, \mathbf{P})$:

$$-\operatorname{div}(\mathbf{a}(x)\nabla U(x, \omega)) = 0, \forall \text{ a.e. } x \in \mathcal{D} \quad (1)$$

with **stochastic Robin** BC (flux $g \in L^2(\partial\mathcal{D})$ given):

$$\mathbf{n}(x)^T \mathbf{a}(x)\nabla U(x, \omega) + \operatorname{Bi}(x, \omega) U(x, \omega) = g(x), \forall \text{ a.e. } x \in \partial\mathcal{D} \quad (2)$$

parametrized by **random input field** $\operatorname{Bi}(x, \omega) \in L^\infty(\partial\mathcal{D}) > 0$.

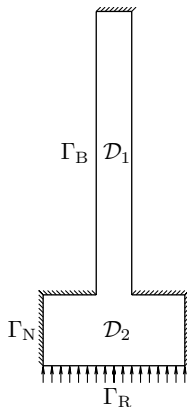
Random output field: $S(\omega) := \mathcal{E}(U(\cdot, \omega)) = \int_{\Gamma_R} U(\cdot, \omega)$

$$\mathbf{E}_{\mathbf{P}}(S(\omega)) = \int_{\Omega} S(\omega) d\mathbf{P}(\omega)$$

$$\operatorname{Var}_{\mathbf{P}}(S(\omega)) = \int_{\Omega} S(\omega)^2 d\mathbf{P}(\omega) - \mathbf{E}_{\mathbf{P}}(S)^2$$

$$\mathbf{a}(x) = \begin{bmatrix} \kappa(x) & 0 \\ 0 & \kappa(x) \end{bmatrix}, \quad \kappa(x) = 1_{\mathcal{D}_1} + \kappa 1_{\mathcal{D}_2}, \quad \forall x \in \mathcal{D}.$$

$$g(x) = 1_{\Gamma_R}, \quad \text{Bi}(x, \omega) = \text{Bi}(x, \omega) 1_{\Gamma_B}, \quad \forall x \in \partial\mathcal{D} \subset (\overline{\Gamma_N} \cup \overline{\Gamma_R} \cup \overline{\Gamma_B}).$$



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Reformulation of the Problem

1. **Karhunen–Loève** (KL) expansion of random input $\text{Bi}(x, \omega)$

$$\text{Bi}(x, \omega) = \mathbf{E}_{\mathbf{P}}(\text{Bi})(x) + \tilde{\Upsilon} \sum_{k=1}^{\mathcal{K}} \sqrt{\lambda_k} \Phi_k(x) Z_k(\omega) ,$$

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- ▶ \mathcal{K} = rank (possibly ∞) of covariance operator for $\text{Bi}(x, \omega)$,
- ▶ with eigenpairs $\left((\tilde{\Upsilon}^2 \lambda_k), \Phi_k(x) \right)_{1 \leq k \leq \mathcal{K}}$,
- ▶ $(Z_k(\omega))_{1 \leq k \leq \mathcal{K}}$ = mutually uncorrelated $L^2_{\mathbf{P}}(\Omega)$ random variables,
- ▶ $\tilde{\Upsilon}$ = positive amplitude parameter.

Reformulation of the Problem

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2. **Truncation** of $\text{Bi}(x, \omega)$ up to order $K \leq \mathcal{K}$: $\text{Bi}_K(x, \omega)$,
→ $\text{Bi}_K(x, \omega)$ instead of $\text{Bi}(x, \omega)$ in (1)–(2)
→ $U_K(x, \omega)$ solution to **new** BVP

Reformulation of the Problem

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2. **Truncation** of $\text{Bi}(x, \omega)$ up to order $K \leq \mathcal{K}$: $\text{Bi}_K(x, \omega)$,
 $\rightarrow U_K(x, \omega)$ solution to **new** BVP
3. $U_K(x, \omega) \sim u_K(x; y^K(\omega))$, $u_K(x; y^K)$ solves **deterministic BVP**

$$-\text{div}(\mathbf{a}(x) \nabla u_K(x; y^K)) = 0 \text{ in } \mathcal{D} \quad (3)$$

$$\mathbf{n}(x)^{\text{T}} \mathbf{a}(x) \nabla u_K(x; y^K) + \text{Bi}_K(x; y^K) u_K(x; y^K) = g(x) \text{ on } \partial \mathcal{D} \quad (4)$$

+ parameter with **law** $y^K := (y_1, \dots, y_K) \sim \tilde{\Upsilon} \sqrt{\lambda_k} (Z_k(\omega))_{1 \leq k \leq K}$.

Computation of statistical outputs

Monte-Carlo (MC) for (many) realizations $S(\omega_m)_{1 \leq m \leq M}$; $M \gg 1$

$$E_M[S_K] = \sum_{m=1}^M \frac{S_K(\omega_m)}{M} \quad V_M[S_K] = \sum_{m=1}^M \frac{(E_M[S_K] - S_K(\omega_m))^2}{M-1}$$

↔

$$E_M[s_K] = \sum_{m=1}^M \frac{s_K(y^K(\omega_m))}{M} \quad V_M[s_K] = \sum_{m=1}^M \frac{(E_M[s_K] - s_K(y^K(\omega_m)))^2}{M-1}$$

where

$\forall y^K, s_K(y^K) = \mathcal{E}(u_K(\cdot; y^K)) \Leftarrow$ **deterministic parametrized BVP**

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where

⇓ **RB**

$\forall y^K, s_K(y^K) = \mathcal{E}(u_K(\cdot; y^K)) \Leftarrow$ **deterministic parametrized BVP**

The Reduced-Basis with output bounds method

1. **Offline:** compute **reduced basis** $\{u_K(\cdot; y_n^K), n = 1 \dots N\}$
for manifold $\{u_K(\cdot; y^K) | y^K \in \text{Range}(y^K)\}$
→ **selection** of parameters $y_n^K \in \text{Range}(y^K)$
in a trial sample of parameters (Greedy procedure or POD).
2. **Online:** compute reduced-basis **approximations**
for **any** $y^K \in \text{Range}(y^K)$
in vector space **Span** $(u_K(\cdot; y_n^K), n = 1 \dots N)$

$$u_K(\cdot; y^K) \simeq u_{N,K}(\cdot; y^K) = \sum_{n=1}^N \alpha_n(y^K) u_K(\cdot; y_n^K)$$

→ coefficients $\alpha_n(y^K)$ *minimize* an **upper bound for output error** in $L^2(\partial\mathcal{D})$.

Rk: parameters y_n^K *maximize* the upper bound for output error.

Benefits of the Reduced-Basis approach

- ▶ MC time computation \searrow (RB = $\frac{1}{50}$ Finite elem. – FE –)
 \uparrow **precomputed reduced basis for $\{u_K(\cdot; y^K)\}$**
- ▶ **no (sensible) loss of accuracy**
 $(|E_M[s_K] - E_M[s_{N,K}]| \leq 0.1\% |E_M[s_{N,K}]|)$
 \uparrow ***a posteriori* bounds for PDE output s_K**
- ▶ + dependence on **additional parameters ϱ ($\neq y^K$)**,
then RB time computation = $\frac{1}{200}$ FE with $\varrho = (\kappa, \overline{\text{Bi}})$

$$\overline{\text{Bi}} := \frac{1}{|\Gamma_B|} \int_{\Gamma_B} \mathbf{E}_P(\text{Bi}) .$$

\uparrow **reduced basis for larger manifold $u_K(\cdot; \varrho, y^K)$**

Relation to Prior Work

Two (expensive) computational approaches:

1. ω -strong

- ▶ simulate probability law $y^K(\omega)$ (low-discrepancy sequences),
- ▶ compute $x \rightarrow u_K(x; y^K(\omega))$ solution to BVP (FE),
- ▶ *large* MC evaluations for moments of $U_K(x, \omega) \sim u_K(x; y^K(\omega))$ (*slow* – statistical – convergence).

2. ω -weak

- ▶ compute $(x, y^K) \rightarrow u_K(x; y^K)$ sol. to *high-dimensional* BVP (x : nodal – FE – basis, y^K : *spectral* – PC – basis [Ghanem-Spanos]),
- ▶ compute moments of $U_K(x, \omega) \sim u_K(x; y^K(\omega))$ through *integral* weighted with *density* of $y^K(\omega)$ (– absolutely continuous – w.r.t. Lebesgue measure on R^K).

Relation to Prior Work

Many reduction attempts:

- ▶ [Schwab, Todor, Frauenfelder ; Wan, Karniadakis]
sparse/adaptive spectral basis for y^K
- ▶ [Babuška, Nobile, Tempone, Webster]
collocation points in $y^K \Rightarrow$ (sparse) – pseudospectral –
orthogonal polynomials
- ▶ [Matthies, Keese]
Krylov iterative method (parallel computers)
- ▶ [Nair, Keane, Sachdeva]
Krylov iterative method (reduced subspace)
- ▶ [Nouy, Le Maître]
generalized spectral decomposition
- ▶ ...

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Random Input Field $B_i(x, \omega)$

1. $B_i(x, \omega) \in L^2(\partial\mathcal{D}, L^2_{\mathbf{p}}(\Omega))$

Random Input Field $\text{Bi}(x, \omega)$

1. $\text{Bi}(x, \omega) \in L^2(\partial\mathcal{D}, L^2_{\mathbf{P}}(\Omega)) \Rightarrow$ KL expansion

$$\text{Bi}(x, \omega) = \mathbf{E}_{\mathbf{P}}(\text{Bi})(x) + \sum_{k=1}^{\mathcal{K}} \sqrt{\tilde{\lambda}_k} \Phi_k(x) Z_k(\omega) . \quad (5)$$

Random Input Field $\text{Bi}(x, \omega)$

1. Proposition: **Hilbert-Schmidt** for (compact) autocovariance

$$\mathbf{Cov}_{\mathbf{P}}(\text{Bi})(x, y) = \int_{\Omega} (\text{Bi}(\omega) - \mathbf{E}_{\mathbf{P}}(\text{Bi}))_x (\text{Bi}(\omega) - \mathbf{E}_{\mathbf{P}}(\text{Bi}))_y d\mathbf{P} .$$

→ complete orthonormal basis $\{\Phi_k(x); k > 0\}$ of $L^2(\partial\mathcal{D}) \ni f$

$$\int_{\partial\mathcal{D}} \mathbf{Cov}_{\mathbf{P}}(\text{Bi})(x, y) f(y) dy = \sum_k \tilde{\lambda}_k \left(\int_{\partial\mathcal{D}} \Phi_k(y) f(y) dy \right) \Phi_k(x) ,$$

→ decorrelated random variables $\mathbf{E}_{\mathbf{P}}(Z_k) = 0$, $\mathbf{Var}_{\mathbf{P}}(Z_k) = 1$ in $L^2_{\mathbf{P}}(\Omega)$

$$Z_k(\omega) = \frac{1}{\sqrt{\tilde{\lambda}_k}} \int_{\partial\mathcal{D}} (\text{Bi} - \mathbf{E}_{\mathbf{P}}(\text{Bi})) \Phi_k, \quad \forall 1 \leq k \leq \mathcal{K} .$$

Random Input Field $B_i(x, \omega)$

1. $B_i(x, \omega) \in L^2(\partial\mathcal{D}, L^2_{\mathbf{P}}(\Omega))$

For practice, rescaling

$$\bar{B}_i := \frac{1}{|\Gamma_B|} \int_{\Gamma_B} \mathbf{E}_{\mathbf{P}}(B_i), \quad \Upsilon := \frac{1}{\bar{B}_i} \sqrt{\int_{\partial\mathcal{D}} \mathbf{Var}_{\mathbf{P}}(B_i)}, \quad \sqrt{\tilde{\lambda}_k} := \frac{\sqrt{\tilde{\lambda}_k}}{\bar{B}_i \Upsilon}$$

so

$$B_i(x, \omega) = \bar{B}_i \left(G(x) + \Upsilon \sum_{k=1}^{\mathcal{K}} \sqrt{\tilde{\lambda}_k} \Phi_k(x) Z_k(\omega) \right). \quad (5)$$

Random Input Field $\text{Bi}(x, \omega)$

1. $\text{Bi}(x, \omega) = \overline{\text{Bi}} \left(G(x) + \Upsilon \sum_k \sqrt{\lambda_k} \Phi_k(x) Z_k(\omega) \right)$
2. $\text{Bi} \in (\bar{b}_{\min}, \bar{b}_{\max})$ a.e. in $\Gamma_B \times \Omega$ ($0 < \bar{b}_{\min} < \bar{b}_{\max} < +\infty$), so
$$\text{Bi}, \text{Bi}^{-1} \in L^\infty(\Gamma_B, L_{\mathbf{P}}^\infty(\Omega)) ;$$

Random Input Field $B_i(x, \omega)$

1. $B_i(x, \omega) = \bar{B}_i (G(x) + \Upsilon \sum_k \sqrt{\lambda_k} \Phi_k(x) Z_k(\omega))$
2. $B_i \in (\bar{b}_{\min}, \bar{b}_{\max})$ a.e. in $\Gamma_B \times \Omega$ ($0 < \bar{b}_{\min} < \bar{b}_{\max} < +\infty$), so

$$B_i, B_i^{-1} \in L^\infty(\Gamma_B, L_{\mathbf{P}}^\infty(\Omega)) ;$$

3. (H1a) $\|\Phi_k\|_{L^\infty(\Gamma_B)} \leq \phi$ (H1b) $\sum_{k=1}^{\mathcal{K}} \sqrt{\lambda_k} < \infty$,
and (H2) $\{Z_k; |Z_k(\omega)| < \sqrt{3}, \mathbf{P}\text{-a.s.}\}$ so

$$\|B_i(x, \omega) - B_{iK}(x, \omega)\|_{L^\infty(\Gamma_B, L_{\mathbf{P}}^\infty(\Omega))} \xrightarrow{K \rightarrow \mathcal{K}} 0, \quad (5)$$

Random Input Field $\text{Bi}(x, \omega)$

- $\text{Bi}(x, \omega) = \bar{\text{Bi}} \left(G(x) + \Upsilon \sum_k \sqrt{\lambda_k} \Phi_k(x) Z_k(\omega) \right)$
- $\text{Bi} \in (\bar{b}_{\min}, \bar{b}_{\max})$ a.e. in $\Gamma_B \times \Omega$ ($0 < \bar{b}_{\min} < \bar{b}_{\max} < +\infty$), so

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- (H1a) $\|\Phi_k\|_{L^\infty(\Gamma_B)} \leq \phi$ (H1b) $\sum_{k=1}^{\mathcal{K}} \sqrt{\lambda_k} < \infty$,
and (H2) $\{Z_k; |Z_k(\omega)| < \sqrt{3}, \mathbf{P}\text{-a.s.}\}$ so

$$\|\text{Bi}(x, \omega) - \text{Bi}_K(x, \omega)\|_{L^\infty(\Gamma_B, L_{\mathbf{P}}^\infty(\Omega))} \xrightarrow{K \rightarrow \mathcal{K}} 0, \quad (5)$$

- (H3) *independent* random variables $\{Z_k\}$,
(H4) $Z_k \sim \mathcal{U}(-\sqrt{3}, \sqrt{3})$, $\forall k$ and (H5) Υ bounded above so

$$\exists \bar{b}_{\min} > 0 / \forall 1 \leq K \leq \mathcal{K}, \text{Bi}_K \geq \bar{b}_{\min} > 0 \text{ a.e. in } \mathcal{D} \times \Omega. \quad (6)$$

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Offline: parameters selection

Offline parameter selection in a **trial sample** $y^K \in \Lambda \subset \text{Range}(y^K)$
→ Greedy procedure (moderate cost):

Step $n = 1 \dots N - 1$, $\{y_i^K \in \Lambda | i = 1 \dots n\}$ already selected:

- ▶ compute RB approximations $\forall y^K \in \Lambda$

$$u_{n,K}(\cdot; y^K) = \sum_{i=1}^n \alpha_i(y^K) u_K(\cdot; y_i^K)$$

- ▶ choose new selection $y_{n+1}^K \in \Lambda$ in

$$\operatorname{argmax} \|s_{n,K} - s_K\|$$

Rk: alternative = POD (more expensive)

A posteriori bounds for outputs

(RB) Approximation error $\|s_{N,K} - s_K\|$

→ *A posteriori* estimation

(between *reduced* $u_{N,K}$ and *very accurate* – FE – $\simeq u_K$)

→ dual norm of the residual error $u_K - u_{N,K}$

+

(KL) Approximation error for output s after truncation

→ *A posteriori* estimation

(between the *very accurate* – FE – $\simeq u_K$ and $\simeq u$)

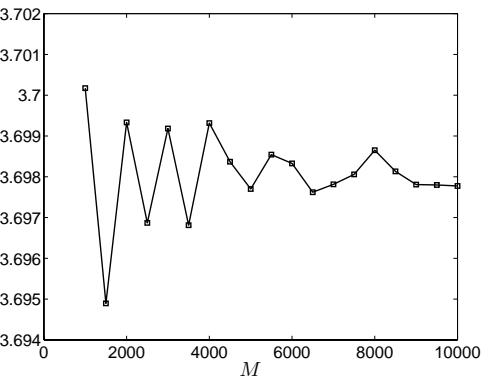
→ $\|B_i - B_{i,K}\|_{L^\infty}$ bounded

Rk: (moderate cost of) online dual norm ← precomputed (linear PDE) Riesz representant (Hilbert)

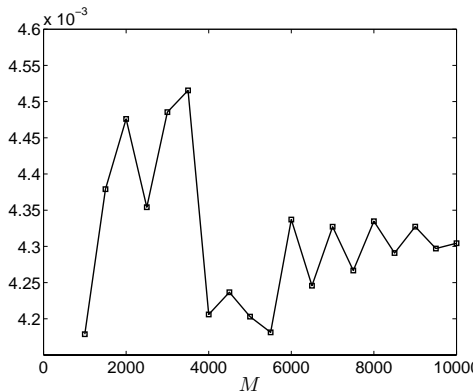
Gaussian covariance kernel for Bi with correlation length δ

$$(\overline{\text{Bi}\Upsilon})^2 e^{-\frac{(x-y)^2}{\delta^2}}$$

(decrease rates of spectrum faster when δ larger)

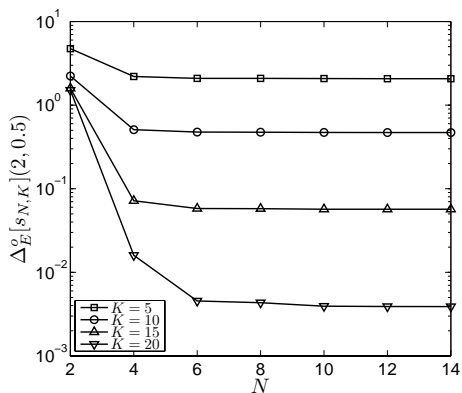


(a) Expected value

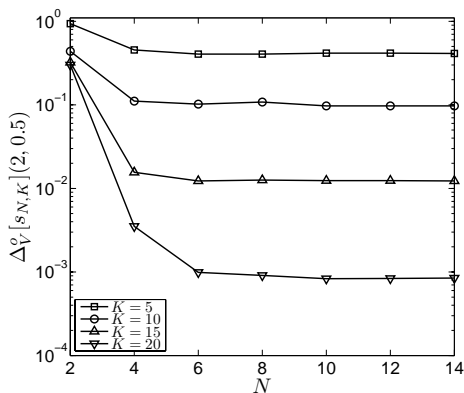


(b) Variance

Figure: Expected value $E_M[s_{N,K}]$ and variance $V_M[s_{N,K}]$ w.r.t. M ($\kappa = 2.0$ and $\overline{\text{Bi}} = 0.5$).

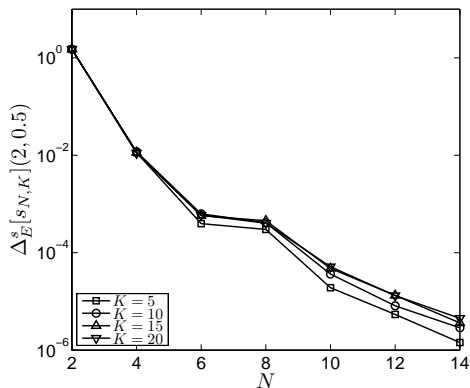


(a)

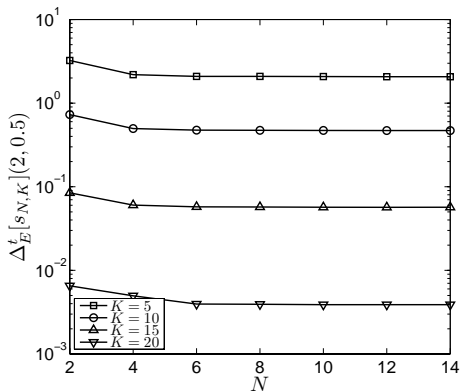


(b)

Figure: Global error bounds for (a) $\mathbf{E}_P(S)$ and (b) $\mathbf{Var}_P(S)$ w.r.t. N and K ($\kappa = 2.0$ and $\overline{\text{Bi}} = 0.5$).

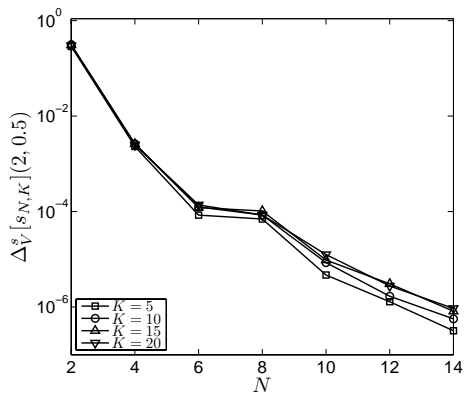


(a)

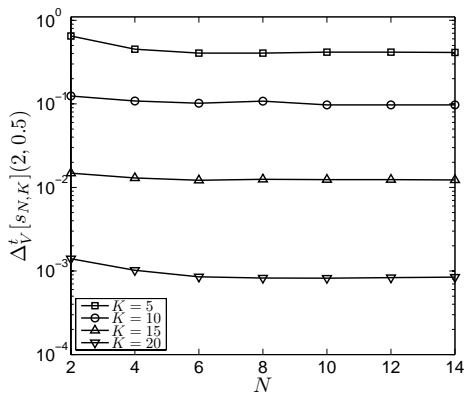


(b)

Figure: Error bounds for $\mathbf{E}_P(S)$ due to (a) approximation in $H^1(\mathcal{D})$ and (b) KL truncation w.r.t. N and K ($\kappa = 2.0$ and $\overline{\text{Bi}} = 0.5$).



(a)



(b)

Figure: Error bounds for $\mathbf{Var}_P(S)$ due to (a) approximation in $H^1(\mathcal{D})$ and (b) KL truncation w.r.t. N and K ($\kappa = 2.0$ and $\overline{\text{Bi}} = 0.5$).

Perspectives:

- ▶ generalization of the method (random input fields)
- ▶ combination with pseudospectral Galerkin method of [Babuška, Nobile, Tempone]

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