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

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Outline of the talk

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

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

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

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

$$-\operatorname{div}\left(\boldsymbol{a}(x)\nabla U(x,\omega)\right) = 0 \ , \forall\, a.e.\, x \in \mathcal{D} \tag{1}$$

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

$$\boldsymbol{n}(x)^{\mathrm{T}}\, \boldsymbol{a}(x)\nabla U(x,\omega) + \mathrm{Bi}(x,\omega)\, U(x,\omega) = g(x) \ , \forall\, a.e.\, x \in \partial\mathcal{D} \tag{2}$$

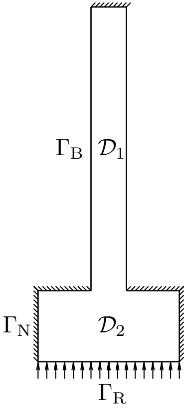
parametrized by random input field $\mathrm{Bi}(x,\omega) \in L^\infty(\partial\mathcal{D}) > 0$.
Random output field: $S(\omega) := \mathcal{E}\left(U(\,\cdot\,,\omega)\right) = \int_{\Gamma_{\mathrm{R}}} U(\,\cdot\,,\omega)$

$$\mathbf{E_P}\left(S(\omega)\right) = \int_\Omega S(\omega)\, d\mathbf{P}(\omega)$$

$$\mathbf{Var_P}\left(S(\omega)\right) = \int_\Omega S(\omega)^2\, d\mathbf{P}(\omega) - \mathbf{E_P}\left(S\right)^2$$

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

$$g(x) = 1_{\Gamma_{\mathrm{R}}} \ , \ \mathrm{Bi}(x,\omega) = \mathrm{Bi}(x,\omega)\, 1_{\Gamma_{\mathrm{B}}} \ , \qquad \forall x \in \partial\mathcal{D} \subset \left(\overline{\Gamma_{\mathrm{N}}} \cup \overline{\Gamma_{\mathrm{R}}} \cup \overline{\Gamma_{\mathrm{B}}}\right) \ .$$



Outline of the talk

Reformulation of the Problem

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

$$\mathrm{Bi}(x,\omega) = \mathbf{E_P}\left(\mathrm{Bi}\right)(x) + \widetilde{\Upsilon} \sum_{k=1}^{\mathcal{K}} \sqrt{\lambda_k} \Phi_k(x) Z_k(\omega) \ ,$$

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

Reformulation of the Problem

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

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

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

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

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

Computation of statistical outputs

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

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

$\hookrightarrow$

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

where

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

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where $\Downarrow$ RB

$\forall y^K,\ s_K(y^K) = \mathcal{E}\left(u_K(\,\cdot\,; y^K)\right) \Leftarrow$ 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 $\{u_K(\cdot\, ; y^K) | y^K \in \mathrm{Range}(y^K)\}$
$\longrightarrow$ *selection* of parameters $y_n^K \in \mathrm{Range}(y^K)$
in a trial sample of parameters (Greedy procedure).
2. Online: compute reduced-basis approximations
for *any* $y^K \in \mathrm{Range}(y^K)$
in vector space **Span** $\left(u_K(\cdot\, ; y_n^K), n = 1 \dots N\right)$

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

$\longrightarrow$ coefficients $\alpha_n(y^K)$ *minimize* an approximation 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
  $(|E_M[s_K] - E_M[s_{N,K}]| \leq 0.1\% |E_M[s_{N,K}]|$ and $\Delta V_M \leq 20\%)$
  $\Uparrow$ *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 $\varrho = (\kappa, \overline{\mathrm{Bi}})$

$$\overline{\mathrm{Bi}} := \frac{1}{|\Gamma_\mathrm{B}|} \int_{\Gamma_\mathrm{B}} \mathbf{E_P}\,(\mathrm{Bi}) \; .$$

$\Uparrow$ 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-discrepency sequences),
   - compute $x \to u_K(x; y^K(\omega))$ 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 $(x, y^K) \to u_K(x; y^K)$ 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
- ...

Outline of the talk

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

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

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

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

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

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

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

$$\mathbf{Cov_P}\left(\mathrm{Bi}\right)(x,y) = \int_\Omega \left(\mathrm{Bi}(\omega) - \mathbf{E_P}\left(\mathrm{Bi}\right)\right)_x \left(\mathrm{Bi}(\omega) - \mathbf{E_P}\left(\mathrm{Bi}\right)\right)_y d\mathbf{P} \ .$$

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

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

$\rightarrow$ decorrelated random variables $\mathbf{E_P}\left(Z_k\right) = 0$, $\mathbf{Var_P}\left(Z_k\right) = 1$ in $L^2_{\mathbf{P}}(\Omega)$

$$Z_k(\omega) = \frac{1}{\sqrt{\tilde{\lambda}_k}} \int_{\partial\mathcal{D}} \left(\mathrm{Bi} - \mathbf{E_P}\left(\mathrm{Bi}\right)\right) \Phi_k, \qquad \forall\, 1 \le k \le \mathcal{K} \ .$$

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

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

   For practice, rescaling

$$\overline{\mathrm{Bi}} := \frac{1}{|\Gamma_B|}\int_{\Gamma_B} \mathbf{E}_{\mathbf{P}}\left(\mathrm{Bi}\right), \Upsilon := \frac{1}{\overline{\mathrm{Bi}}}\sqrt{\int_{\partial\mathcal{D}} \mathbf{Var}_{\mathbf{P}}\left(\mathrm{Bi}\right)}, \sqrt{\lambda_k} := \frac{\sqrt{\tilde{\lambda}_k}}{\overline{\mathrm{Bi}}\Upsilon}$$

so

$$\mathrm{Bi}(x,\omega) = \overline{\mathrm{Bi}}\left(G(x) + \Upsilon \sum_{k=1}^{\mathcal{K}} \sqrt{\lambda_k}\,\Phi_k(x)\, Z_k(\omega)\right) . \qquad (5)$$

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

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

$$\mathrm{Bi}, \mathrm{Bi}^{-1} \in L^\infty\left(\Gamma_{\mathrm{B}}, L^\infty_{\mathbf{P}}(\Omega)\right) \;;$$

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

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$$\mathrm{Bi}, \mathrm{Bi}^{-1} \in L^\infty\left(\Gamma_{\mathrm{B}}, L^\infty_{\mathbf{P}}(\Omega)\right) \ ;$$

3. (H1a) $\|\Phi_k\|_{L^\infty(\Gamma_{\mathrm{B}})} \leq \phi$ (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

$$\|\mathrm{Bi}(x,\omega) - \mathrm{Bi}_K(x,\omega)\|_{L^\infty(\Gamma_{\mathrm{B}}, L^\infty_{\mathbf{P}}(\Omega))} \xrightarrow{K \to \mathcal{K}} 0 \ , \qquad (5)$$

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

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2. $\mathrm{Bi} \in (\bar{b}_{\min}, \bar{b}_{\max})$ a.e. in $\Gamma_{\mathrm{B}} \times \Omega$ $(0 < \bar{b}_{\min} < \bar{b}_{\max} < +\infty)$, so
$$\mathrm{Bi}, \mathrm{Bi}^{-1} \in L^\infty\left(\Gamma_{\mathrm{B}}, L^\infty_{\mathbf{P}}(\Omega)\right) \ ;$$
3. (H1a) $\|\Phi_k\|_{L^\infty(\Gamma_{\mathrm{B}})} \le \phi$ (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
$$\left\|\mathrm{Bi}(x,\omega) - \mathrm{Bi}_K(x,\omega)\right\|_{L^\infty(\Gamma_{\mathrm{B}}, L^\infty_{\mathbf{P}}(\Omega))} \xrightarrow{K \to \mathcal{K}} 0 \ , \qquad (5)$$
4. (H3) *independent* random variables $\{Z_k\}$,
(H4) $Z_k \sim \mathcal{U}(-\sqrt{3}, \sqrt{3})$, $\forall k$ and (H5) Υ bounded above so
$$\exists \bar{b}_{min} > 0 \ / \ \forall 1 \le K \le \mathcal{K},\ \mathrm{Bi}_K \ge \bar{b}_{\min} > 0 \text{ a.e. in} \mathcal{D} \times \Omega. \quad (6)$$

Outline of the talk

Offline: parameters selection

Offline parameter selection in a trial sample $y^K \in \Lambda \subset \mathrm{Range}(y^K)$
$\longrightarrow$ 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

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

Rk: alternative = POD (more expensive, not hierarchical)

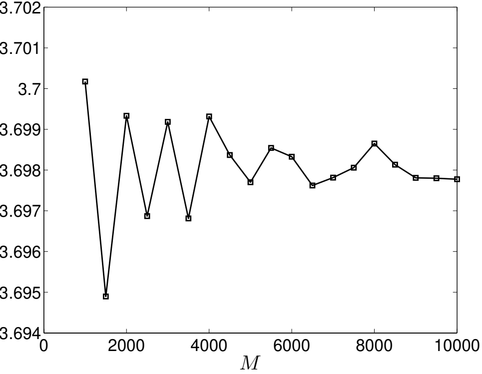
A posteriori bounds for outputs

(RB) Approximation error $\|s_{N,K} - s_K\|$
$\longrightarrow$ *A posteriori* estimation
(between *reduced* $u_{N,K}$ and *very accurate* – FE – $\simeq u_K$)
$\longrightarrow$ dual norm of the residual error $u_K - u_{N,K}$
$+$
(KL) Approximation error for output s after truncation
$\longrightarrow$ *A posteriori* estimation
(between the *very accurate* – FE – $\simeq u_K$ and $\simeq u$)
$\longrightarrow$ $\|\mathrm{Bi} - \mathrm{Bi}_K\|_{L^\infty}$ bounded
Rk: (moderate cost of) online dual norm $\longleftarrow$ precomputed (linear PDE) Riesz representant (Hilbert)

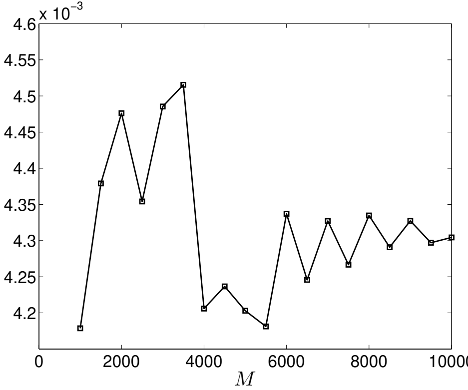
Gaussian covariance kernel for Bi with correlation length δ

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

(decrease rates of spectrum faster when δ larger)
$\delta = 0.5$ and $K \leq 25 \to \Upsilon \leq 0.058$ and $N = 18$
$\delta = 0.2$ and $K \leq 60 \to \Upsilon \leq 0.074$ and $N = 32$
(greedy stops when maximal error bound is less than 10^{-3})

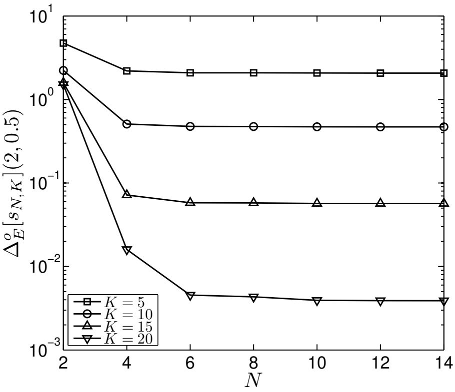


(a) Expected value

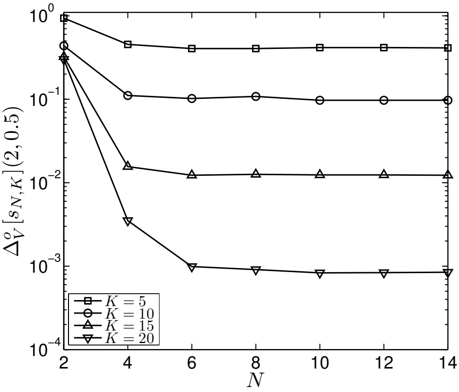


(b) Variance

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



(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 $\overline{\mathrm{Bi}} = 0.5$).

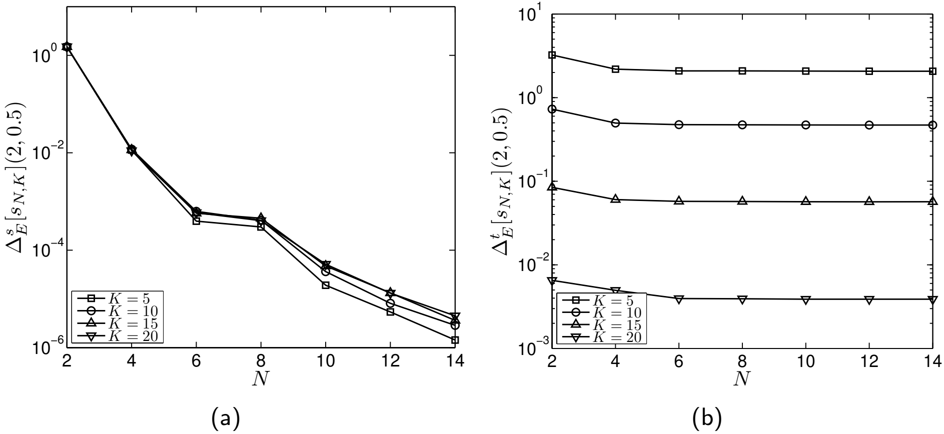
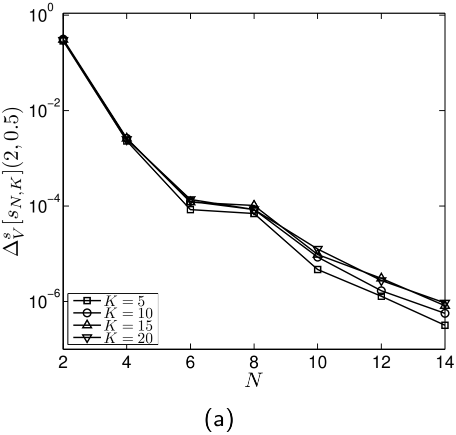


Figure: Error bounds for $\mathbf{E_P}(S)$ due to (a) approximation in $H^1(\mathcal{D})$ and (b) KL truncation w.r.t. N and K ($\kappa = 2.0$ and $\overline{\mathrm{Bi}} = 0.5$).



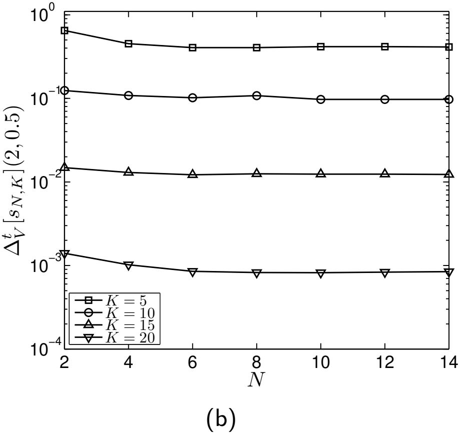


Figure: Error bounds for $\mathbf{Var_P}(S)$ due to (a) approximation in $H^1(\mathcal{D})$ and (b) KL truncation w.r.t. N and K ($\kappa = 2.0$ and $\overline{\mathrm{Bi}} = 0.5$).

Perspectives:

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

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