Stochastic Galerkin reduced basis methods for parametrized linear elliptic PDEs*

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Abstract. We consider the estimation of parameter-dependent statistics of functional outputs of elliptic boundary value problems with parametrized random and deterministic inputs. For a given value of the deterministic parameter, a stochastic Galerkin finite element (SGFE) method can estimate the corresponding expectation and variance of a linear output at the cost of a single solution of a large block-structured linear algebraic system of equations. We propose a stochastic Galerkin reduced basis (SGRB) method as a means to lower the computational burden when statistical outputs are required for a large number of deterministic parameter queries. To derive an SGRB model, we project the spatial-stochastic weak solution of a parameter-dependent SGFE model onto a POD reduced basis generated from snapshots of the SGFE solution at representative values of the parameter. We propose residual-corrected estimates of the parameter-dependent expectation and variance of linear functional outputs and provide respective computable error bounds. We test the SGRB method numerically for a convection-diffusion-reaction problem, choosing the convective velocity as a deterministic parameter and the parametrized reactivity field as a random input. Compared to a standard reduced basis model embedded in a Monte Carlo sampling procedure, the SGRB model requires a similar number of reduced basis functions to meet a given tolerance requirement. However, only a single run of the SGRB model suffices to estimate a statistical output for a new deterministic parameter value, while the standard reduced basis model must be solved for each Monte Carlo sample.

Key words. Model order reduction, reduced basis method, stochastic Galerkin, finite elements, parametrized partial differential equation, Monte Carlo, proper orthogonal decomposition.

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- 1. Introduction. We consider linear elliptic boundary-value problems subject to a finite number of random and deterministic input parameters. We are interested in computing the parameter-dependent expected value and variance of a functional output of interest. In this context, a reduced basis model provides a computationally inexpensive map between the deterministic input parameter and the corresponding output statistics. Moreover, it provides a computable a posteriori bound for the error between the reduced basis statistical estimate and a corresponding high-fidelity estimate. Reduced basis methods for linear elliptic boundary value problems with affinely parametrized deterministic data are well-understood [12, 20, 22]. We consider two approaches to including stochastic parameters:
 - Monte Carlo reduced basis (MCRB) method: The underlying equations are formulated

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weakly regarding the physical space, which means that the problem depends on both the deterministic and stochastic parameters. Monte Carlo sampling is used to estimate the parameter-dependent expected value and variance of a functional output. An MCRB method for linear elliptic problems with error bounds for the expectation and variance of a linear functional output is derived in [3]. Improved error bounds are provided by [11]. Further advances are the introduction of a weighted error estimator [5] and the embedding in a multi-level procedure [28]. MCRB methods have also been applied to parabolic problems [24], saddle point problems [16], Bayesian inverse problems [2, 6, 15] and the assessment of rare events [4].

• Stochastic Galerkin reduced basis (SGRB) method: The underlying equations are formulated weakly regarding the spatial and stochastic dimensions, so that the problem depends on the deterministic parameters, only. Parameter-dependent estimates of the expected value and variance of a functional output are obtained by direct integration of the reduced solution. The principle of SGRB methods is introduced in [27] for stochastic time-dependent incompressible Navier-Stokes problems, formulated weakly regarding the spatial and stochastic dimensions, with time acting as a parameter. Applications to linear dynamical systems are studied in [8, 21]. SGRB methods can be related to space-time reduced basis methods [10, 26], which rely on a weak formulation with respect to space and time. The idea of using SGRB methods to estimate parameter-dependent expected values is discussed in [29, section 8.2.1].

Our main contribution is the derivation of a stochastic Galerkin reduced basis method to compute residual-corrected parameter-dependent estimates of the expectation and variance of statistical outputs together with corresponding error bounds. A Monte Carlo reduced basis method will be used as a benchmark to assess the accuracy of the SGRB method and compare the error bounds.

The creation of a Stochastic Galerkin reduced basis model requires an underlying stochastic Galerkin finite element (SGFE) model or an equivalent high-fidelity Galerkin approximation. At least a few snapshots of the SGFE solution for different values of the deterministic parameter are needed to provide a suitable reduced basis. Moreover, evaluations of the SGFE linear and bilinear forms are necessary to derive the respective reduced-order Galerkin model and error bounds. Therefore, the SGRB method can not reduce the computational burden associated with a single solution of an SGFE model, as done in [18, 25] using proper generalized decomposition and in [19] using a rational Krylov method. Instead, the method targets the situation where a few SGFE simulations are feasible in an expensive pre-processing step to create a reduced-order model which can be evaluated cheaply for any given deterministic parameter. Therefore, SGRB models can be particularly useful in settings where statistical estimates are required for many values of the deterministic parameter, like in robust optimal control or the real-time exploration of parameter-dependent statistics.

Compared to Monte Carlo reduced basis methods, stochastic Galerkin reduced basis methods can substantially decrease the computational cost of estimating the expectation and variance for a given deterministic parameter value. The reason is that MCRB methods require sampling the reduced-order solution, which may lead to a large number of reduced-order simulations for a single query of the deterministic parameter. SGRB methods overcome this drawback by evaluating the stochastic integrals in the offline stage, i.e., during the setup of

the reduced-order model. As a result, the cost of solving an SGRB model is similar to the cost of a single solution of a comparable RB model within an MC loop. At the same time, the SGRB model directly delivers a statistical estimate without sampling. Therefore, one can expect a speed-up factor in the order of magnitude of the number of MC samples.

2. Monte Carlo reduced basis method. We introduce a complete probability space $(\Theta, \mathcal{F}, \mathbb{P})$ consisting of a set Θ of elementary events, a σ -algebra \mathcal{F} on Θ and a probability measure \mathbb{P} on \mathcal{F} . For $k=1,\ldots,K$ with $K\in\mathbb{N}$, we define independent random variables $\xi_k\colon\Theta\to\Xi_k$, where $\Xi_k\subset\mathbb{R}$ is the image of ξ_k . We introduce respective probability distributions \mathbb{P}_{ξ_k} and probability densities $p_{\xi_k}:\Xi_k\to\mathbb{R}^+$, so that $\mathbb{P}_{\xi_k}(B)=\int_B p_{\xi_k}(y)\,\mathrm{d}y=\mathbb{P}(\xi_k^{-1}(B))$ for all B in the Borel σ -algebra of Ξ_k . We collect the random variables in a random vector $\xi\colon\Theta\to\Xi$, where $\xi=(\xi_1,\ldots,\xi_K)^T$ and $\Xi=\Xi_1\times\cdots\times\Xi_K$, with joint distribution \mathbb{P}_ξ and density $p_\xi:\Xi\to\mathbb{R}^+$. We denote the expectation of any \mathbb{P}_ξ -measurable function $g\colon\Xi\to\mathbb{R}$ with density p_ξ by $\mathbb{E}[g]=\int_\Xi g(y)\,\mathrm{d}\mathbb{P}_\xi(y)=\int_\Xi g(y)p_\xi(y)\,\mathrm{d}y$. We define the variance $\mathbb{V}[g]=\mathbb{E}[(g-\mathbb{E}[g])^2]$ for any $g\in L_\xi^2(\Xi)$, where $L_\xi^2(\Xi):=\{v:\Xi\to\mathbb{R}\mid \int_\Xi v(y)^2p_\xi(y)\,\mathrm{d}y<\infty\}$.

We introduce a deterministic parameter $\mu \in \mathcal{P}$ for some parameter domain $\mathcal{P} \subset \mathbb{R}^P$ with $P \in \mathbb{N}$. The final statistical outputs are scalar-valued μ -dependent functions representing approximations to the expectation and variance of a linear functional of a PDE solution.

We let $\{\xi^1,\ldots,\xi^{N_\xi}\}$ be a set of independent copies of the random vector ξ . For some $g\in L^2_{\xi}(\Xi)$, we define Monte Carlo estimators

(1)
$$E[g] := \frac{1}{N_{\xi}} \sum_{n=1}^{N_{\xi}} g(\xi^n), \quad \underline{E}[g] := \frac{1}{N_{\xi} - 1} \sum_{n=1}^{N_{\xi}} g(\xi^n), \quad V[g] := \underline{E}[g^2] - \underline{E}[g]E[g],$$

for which $\mathbb{E}[E[g]] = \mathbb{E}[g]$ and $\mathbb{E}[V[g]] = \mathbb{V}[g]$ hold. We let $\Xi^{N_{\xi}} := \{y^1, \dots, y^{N_{\xi}}\}$ be a realization of $\{\xi^1, \dots, \xi^{N_{\xi}}\}$. A realization of a Monte Carlo estimate is obtained after substituting ξ^n by y^n in (1), assuming that g(y) is computable for any $y \in \Xi^{N_{\xi}}$. In our approach, we view N_{ξ} as a discretization parameter and fix $\Xi^{N_{\xi}}$ before we build the reduced basis model.

We focus on the case where g depends on its argument via a discretized PDE problem. In the following, we provide a full-order model (subsection 2.1) and a reduced-order model (subsection 2.2) to approximate the solution of the PDE for a given realization of the deterministic and random input parameters. The computation of linear outputs and the corresponding statistics are described in subsection 2.3, together with the respective error bounds. For the separation of the computation into an expensive offline phase and a inexpensive online phase, we refer to [3, 11].

2.1. Monte Carlo finite element model. We use a stochastic strong form of a parametrized PDE problem with random data to formulate an MCFE model. Samples of the solution of the PDE problem are characterized by a separable Hilbert space X with inner product $(\cdot, \cdot)_X$ and norm $\|\cdot\|_X$. We introduce a parametrized bilinear form $a(\cdot, \cdot; y, \mu) : X \times X \to \mathbb{R}$ as well as a parametrized linear form $f(\cdot; y, \mu) : X \to \mathbb{R}$. This allows a stochastic strong formulation of a linear elliptic PDE problem:

Problem 2.1 (MCFE model). For given $(y, \mu) \in \Xi^{N_{\xi}} \times \mathcal{P}$, find

(2)
$$u(y,\mu) \in X : a(u(y,\mu), v; y, \mu) = f(v; y, \mu) \quad \forall v \in X.$$

We assume that $a(\cdot, \cdot; y, \mu)$ is (y, μ) -uniformly bounded and coercive on X and that $f(\cdot; y, \mu)$ is (y, μ) -uniformly bounded on X. Then Problem 2.1 has a unique solution for any given $(y, \mu) \in \Xi^{N_{\xi}} \times \mathcal{P}$ according to the Lax-Milgram lemma.

It is a usual premise in reduced basis methods that the discretization space of the underlying full-order model is assumed to be large enough to capture the solution with sufficient precision. The assessment of the error of the full-order solution with respect to the infinite-dimensional exact solution is delegated to the choice of the full-order discretization. In this spirit, we assume X to be a sufficiently well-resolving finite element space with $M_{\rm FE}$ degrees of freedom. Similarly, we assume $\Xi^{N_{\xi}}$ to be a large enough sample set, so that the error associated with the MC sampling is sufficiently small. Consequently, the errors associated with the MC sampling and the FE discretization are not represented in our error estimates.

2.2. Monte Carlo reduced basis model. Let $X^R \subset X$ be an R-dimensional subspace. An example is given in subsection 4.1. A reduced-order model of Problem 2.1 is

Problem 2.2 (MCRB model). For given
$$(y,\mu) \in \Xi^{N_{\xi}} \times \mathcal{P}$$
, find
$$u^{R}(y,\mu) \in X^{R}: \quad a(u^{R}(y,\mu),v;y,\mu) = f(v;y,\mu) \quad \forall v \in X^{R}.$$

The unique solvability if Problem 2.2 is a direct consequence of Problem 2.1 being well-posed and X^R being a subspace of X.

2.3. Output statistics and error estimates. We derive residual-corrected RB approximations of MCFE estimates of the expectation and variance of linear outputs of the parametrized PDE problem. We provide error bounds converging quadratically in terms of residual norms. In particular, we transfer the dual-based error bounds of [11], considering the *true* expectation and variance of RB outputs, to the setting of [3], considering MC approximations of the expectation and variance. This requires an additional dual problem as well as a careful handling of different MC discretizations of the expected value, namely $E[\cdot]$ and $E[\cdot]$ according to (1). Throughout this section, we assume the same dependency on the deterministic and stochastic parameters as in subsections 2.1 and 2.2, but often omit an explicit notation of the parameter dependence for clarity.

We introduce a parametrized linear form $l(\cdot; y, \mu) : X \to \mathbb{R}$, assumed to be (y, μ) -uniformly bounded on X. We complement Problems 2.1 and 2.2 with auxiliary sets of dual problems to allow for residual-corrected output computations. For brevity, we provide the definitions and problems all at once, which results in some interconnections between the following statements:

Definition 2.3. Subspaces $X_{(1)}^R, \ldots, X_{(4)}^R$ and linear forms $l_{(1)}, \ldots, l_{(4)}$ are given by

$$\begin{split} X^R_{(1)} \subset X, & l_{(1)}(\cdot) := l(\cdot), \\ X^R_{(2)} \subset X, & l_{(2)}(\cdot) := 2(l(u^R) - r(u^R_{(1)}))l(\cdot), \\ X^R_{(3)} \subset X, & l_{(3)}(\cdot) := E[l(u^R) - r(u^R_{(1)})]l(\cdot), \\ X^R_{(4)} \subset X, & l_{(4)}(\cdot) := \underline{E}[l(u^R) - r(u^R_{(1)})]l(\cdot). \end{split}$$

Problem 2.4 (dual MCFE models). For given $(y, \mu) \in \Xi^{N_{\xi}} \times \mathcal{P}$, find

$$u_{(i)} \in X : \quad a(v, u_{(i)}) = -l_{(i)}(v) \quad \forall v \in X, \quad i = 1, \dots, 4.$$

Problem 2.5 (dual MCRB models). For given $(y, \mu) \in \Xi^{N_{\xi}} \times \mathcal{P}$, find

$$u_{(i)}^R \in X_{(i)}^R$$
: $a(v, u_{(i)}^R) = -l_{(i)}(v) \quad \forall v \in X_{(i)}^R$, $i = 1, \dots, 4$.

Definition 2.6. A primal residual r and dual residuals $r_{(1)}, \ldots, r_{(4)}$ are given by

(3)
$$r(\cdot) := f(\cdot) - a(u^R, \cdot),$$

(4)
$$r_{(i)}(\cdot) := -l_{(i)}(\cdot) - a(\cdot, u_{(i)}^R), \quad i = 1, \dots 4.$$

The following error bounds require a coercivity factor

(5)
$$\alpha(y,\mu) := \inf_{v \in X \setminus \{0\}} \frac{a(v,v;y,\mu)}{\|v\|_Y^2} \quad \forall (y,\mu) \in \Xi^{N_{\xi}} \times \mathcal{P},$$

and a dual space X' of X, with norm

(6)
$$||F||_{X'} := \sup_{v \in X \setminus \{0\}} \frac{|F(v)|}{||v||_X} \quad \forall F \in X'.$$

For efficiency, an offline/online decomposition of the dual norms of the encountered functional is possible and the coercivity factor can be replaced by a strictly positive lower bound [3, 11].

First, we provide a bound for the error of the RB solution to Problem 2.2 with respect to the FE solution to Problem 2.1, point-wise in $\Xi^{N_{\xi}} \times \mathcal{P}$, see [11, Proposition 3.1]:

Lemma 2.7 (solution bound). For given $(y, \mu) \in \Xi^{N_{\xi}} \times \mathcal{P}$,

(7)
$$||u - u^R||_X \le \frac{||r||_{X'}}{\alpha}.$$

Proof. We define $e := u - u^R$ and derive

$$\alpha \|e\|_X^2 \stackrel{(5)}{\leq} a(e,e) \stackrel{(2)}{=} f(e) - a(u^R,e) \stackrel{(3)}{=} r(e) \stackrel{(6)}{\leq} \|r\|_{X'} \|e\|_X.$$

Dividing by $\alpha ||e||_X$ gives the result.

We approximate a parameter-dependent linear output $l(u(y, \mu); y, \mu)$ point-wise with a residual-corrected reduced-order approximation, see [11, Theorem 3.6]:

Lemma 2.8 (output bound). For given $(y, \mu) \in \Xi^{N_{\xi}} \times \mathcal{P}$,

(8)
$$|l(u) - l(u^R) + r(u_{(1)}^R)| \le \frac{||r||_{X'} ||r_{(1)}||_{X'}}{\alpha}.$$

Proof. We define $e := u - u^R$ and reformulate

$$\begin{aligned} |l(u) - l(u^R) + r(u_{(1)}^R)| &\stackrel{(3)}{=} |l(e) + f(u_{(1)}^R) - a(u^R, u_{(1)}^R)| \stackrel{(2)}{=} |l(e) + a(e, u_{(1)}^R)| \\ &\stackrel{(4)}{=} |r_{(1)}(e)| \stackrel{(6)}{\leq} ||r_{(1)}||_{X'} ||e||_X \stackrel{(7)}{\leq} \frac{||r_{(1)}||_{X'} ||r||_{X'}}{\alpha}. \end{aligned}$$

We approximate the MCFE estimate $E[l(u(\cdot, \mu); \cdot, \mu)]$ of the parameter-dependent expected linear output as follows, see [11, Corollary 4.2.]:

Theorem 2.9 (expected output bound). For given $\mu \in \mathcal{P}$,

$$|E[l(u)] - E[l(u^R)] + E[r(u_{(1)}^R)]| \le E\left[\frac{||r||_{X'}||r_{(1)}||_{X'}}{\alpha}\right].$$

Proof. By Jensen's inequality

$$|E[l(u)] - E[l(u^R)] + E[r(u_{(1)}^R)]| \le E[|l(u) - l(u^R) + r(u_{(1)}^R)|] \le E\left[\frac{||r||_{X'}||r_{(1)}||_{X'}}{\alpha}\right].$$

Finally, we approximate the MCFE estimate $V[l(u(\cdot, \mu); \cdot, \mu)]$ of the parameter-dependent variance of the linear output, see [11, Theorem 4.5]:

Theorem 2.10 (output variance bound). For given $\mu \in \mathcal{P}$,

$$\begin{split} \left| V[l(u)] - V[l(u^R)] + V[r(u_{(1)}^R)] + \underline{E}[r(u_{(2)}^R)] - \underline{E}[r(u_{(3)}^R)] - E[r(u_{(4)}^R)] \right| \\ & \leq \underline{E} \left[\frac{\|r\|_{X'}^2 \|r_{(1)}\|_{X'}^2}{\alpha^2} \right] + E \left[\frac{\|r\|_{X'} \|r_{(1)}\|_{X'}}{\alpha} \right] \underline{E} \left[\frac{\|r\|_{X'} \|r_{(1)}\|_{X'}}{\alpha} \right] \\ & + \underline{E} \left[\frac{\|r_{(2)} - r_{(3)} - \frac{N_{\xi} - 1}{N_{\xi}} r_{(4)}\|_{X'} \|r\|_{X'}}{\alpha} \right]. \end{split}$$

Proof. By (1), defining $e := u - u^R$,

$$\begin{split} & |\underline{E}[l(u)^2] - \underline{E}[l(u)]E[l(u)] - \underline{E}[l(u^R)^2] + \underline{E}[l(u^R)]E[l(u^R)] \\ & + \underline{E}[r(u^R_{(1)})^2] - \underline{E}[r(u^R_{(1)})]E[r(u^R_{(1)})] + \underline{E}[r(u^R_{(2)})] - \underline{E}[r(u^R_{(3)})] - E[r(u^R_{(4)})]| \\ & \leq \underline{|\underline{E}[(l(u) - l(u^R) + r(u^R_{(1)}))^2]|} \\ & + \underline{|\underline{E}[l(u) - l(u^R) + r(u^R_{(1)})]|} \underline{|\underline{E}[l(u) - l(u^R) + r(u^R_{(1)})]|} \\ & + \underline{|\underline{E}[l(u) - l(u^R) + r(u^R_{(1)})]|} \underline{|\underline{E}[l(u) - l(u^R) + r(u^R_{(1)})]|} \\ & + \underline{|\underline{E}[l(u) - l(u^R) + r(u^R_{(1)})]|} \\ & + \underline{|\underline{E}[l(u^R) - r(u^R_{(1)})] |\underline{e}]} \\ & + \underline{|\underline{E}[l(u^R) - r(u^R_{(1)})] |\underline{e}]} \\ & + \underline{|\underline{E}[l(u^R) - r(u^R_{(1)})] |\underline{e}]} \\ & - \underline{E}[\underline{[l(u^R) - r(u^R_{(1)})] |\underline{e}]} \\ & - \underline{E}[\underline{[l(u^R) - r(u^R_{(1)})] |\underline{e}]} \\ & - \underline{E}[\underline{[l(u^R) - r(u^R_{(1)})] |\underline{e}]}] \\ & + \underline{|\underline{E}[l(u^R) - r(u^R_{(1)})] |\underline{e}]} \\ & + \underline{|\underline{E}[l(u^R) - r(u^R_{(1)})] |\underline{e}]} \\ & - \underline{|\underline{E}[l(u^R) - r(u^R_{(1)})] |\underline{e}]} \\ & + \underline{|\underline{E}[l(u^R) - r(u^R_{(1)})]} \\ & + \underline{|\underline{E}[l(u^R) - r(u^R_{(1)})]} \\ & + \underline{|\underline{E}[l(u^R) - r(u^R_{(1)})]} \\ & + \underline{|\underline{E}[l(u^$$

where

$$\left| \underline{E}[r_{(2)}(e)] - \underline{E}[r_{(3)}(e)] - E[r_{(4)}(e)] \right| \stackrel{(6),(7)}{\leq} \underline{E} \left[\frac{\|r_{(2)} - r_{(3)} - \frac{N_{\xi} - 1}{N_{\xi}} r_{(4)} \|_{X'} \|r\|_{X'}}{\alpha} \right].$$

- 3. Stochastic Galerkin reduced basis method. In the following, we replace the Monte Carlo sampling by a stochastic Galerkin procedure. We provide a full-order model (subsection 3.1) and a reduced-order model (subsection 3.2) to approximate the stochastic solution of the PDE problem for a given realization of the deterministic input parameters. The computation of statistics of linear outputs are described in subsection 3.3, together with the respective error bounds. The computation can be separated into an expensive offline phase and a inexpensive online phase by standard means [20].
- **3.1. Stochastic Galerkin finite element model.** We introduce a stochastic Galerkin discretization space $S \subset L^2_{\xi}(\Xi)$. An example is given in subsection 5.2. We define the product space $\bar{X} := S \otimes X$, which is a Hilbert space with inner product $(\cdot, \cdot)_{\bar{X}} := (\cdot, \cdot)_{L^2_{\xi}(\Xi, X)}$ and norm $\|\cdot\|_{\bar{X}} := \|\cdot\|_{L^2_{\xi}(\Xi, X)}$ in terms of $L^2_{\xi}(\Xi, X) := \{v : \Xi \to X \mid \int_{\Xi} \|v(y)\|_X^2 p_{\xi}(y) \, \mathrm{d}y < \infty \}$.

We derive a stochastic weak form by taking the expectation of (2). Defining $\bar{a}(w, v; \mu) := \mathbb{E}[a(w, v; \cdot, \mu)]$ and $\bar{f}(v; \mu) := \mathbb{E}[f(v; \cdot, \mu)]$ provides

Problem 3.1 (SGFE model). For given $\mu \in \mathcal{P}$, find

(9)
$$\bar{u}(\mu) \in \bar{X} : \bar{a}(\bar{u}(\mu), v; \mu) = \bar{f}(v; \mu) \quad \forall v \in \bar{X}.$$

As a consequence of the coercivity and boundedness properties associated with Problem 2.1, the bilinear form $\bar{a}(\cdot,\cdot;\mu)$ is μ -uniformly bounded and coercive on \bar{X} and the linear form $\bar{f}(\cdot;\mu)$ is μ -uniformly bounded on \bar{X} . Therefore, Problem 3.1 has a unique solution for any given $\mu \in \mathcal{P}$ according to the Lax-Milgram lemma.

3.2. Stochastic Galerkin reduced basis model. We introduce an R-dimensional reduced space $\bar{X}^R \subset \bar{X}$. Suitable reduced spaces are provided in subsection 4.2. A reduced form of Problem 3.1 is given as follows:

Problem 3.2 (SGRB model). For given $\mu \in \mathcal{P}$, find

$$\bar{u}^R(\mu) \in \bar{X}^R : \quad \bar{a}(\bar{u}^R(\mu), v; \mu) = \bar{f}(v; \mu) \quad \forall v \in \bar{X}^R.$$

The subspace property $\bar{X}^R \subset \bar{X}$ and the well-posedness of Problem 3.1 imply that Problem 3.2 has a unique solution.

3.3. Output statistics and error estimates. We derive SGRB approximations of the expectation and variance of linear outputs together with error bounds with respect to the corresponding SGFE approximations. The variance can be interpreted in terms of quadratic outputs. We follow the ideas of [13, 23] to derive the respective error bounds.

We introduce a linear form $\bar{l}(v;\mu) := \mathbb{E}[l(v;\cdot,\mu)]$, which is μ -uniformly bounded on \bar{X} . We complement the primal problem of subsection 3.1 with corresponding dual problems:

Problem 3.3 (dual SGFE models). For given $\mu \in \mathcal{P}$, find

$$\begin{split} \bar{u}_{(1)} \in \bar{X} \ : \quad & \bar{a}(v, \bar{u}_{(1)}) = -\bar{l}(v) \\ \bar{u}_{(2)} \in \bar{X} \ : \quad & \bar{a}(v, \bar{u}_{(2)}) = -\mathbb{E}[l(\bar{u} + \bar{u}^R)l(v)] \\ \bar{u}_{(3)} \in \bar{X} \ : \quad & \bar{a}(v, \bar{u}_{(3)}) = -(\bar{l}(\bar{u}) + \bar{l}(\bar{u}^R) - 2\bar{r}(\bar{u}^R_{(1)}))\bar{l}(v) \end{split} \quad \forall v \in \bar{X}.$$

Letting $\bar{X}^R_{(1)} \subset \bar{X}$, $\bar{X}^R_{(2)} \subset \bar{X}$ and $\bar{X}^R_{(3)} \subset \bar{X}$ be R-dimensional subspaces, we introduce the following set of reduced dual equations:

Problem 3.4 (dual SGRB models). For given $\mu \in \mathcal{P}$, find

$$\begin{split} \bar{u}^R_{(1)} \in \bar{X}^R_{(1)} : \quad \bar{a}(v, \bar{u}^R_{(1)}) = -\bar{l}(v) & \forall v \in \bar{X}^R_{(1)}, \\ \bar{u}^R_{(2)} \in \bar{X}^R_{(2)} : \quad \bar{a}(v, \bar{u}^R_{(2)}) = -2\mathbb{E}[l(\bar{u}^R)l(v)] & \forall v \in \bar{X}^R_{(2)}, \\ \bar{u}^R_{(3)} \in \bar{X}^R_{(3)} : \quad \bar{a}(v, \bar{u}^R_{(3)}) = -2\big(\bar{l}(\bar{u}^R) - \bar{r}(\bar{u}^R_{(1)})\big)\bar{l}(v) & \forall v \in \bar{X}^R_{(3)}. \end{split}$$

The error bounds will be provided in terms of dual norms of residuals:

Definition 3.5. Based on Problems 3.1 to 3.4,

(10)
$$\bar{r}(\cdot) := \bar{f}(\cdot) - \bar{a}(\bar{u}^R, \cdot),$$

(11)
$$\bar{r}_{(1)}(\cdot) := -\bar{l}(\cdot) - \bar{a}(\cdot, \bar{u}_{(1)}^R),$$

(12)
$$\bar{r}_{(2)}(\cdot) := -2\mathbb{E}[l(\bar{u}^R)l(\cdot)] - \bar{a}(\cdot, \bar{u}_{(2)}^R),$$

(13)
$$\bar{r}_{(3)}(\cdot) := -2(\bar{l}(\bar{u}^R) - \bar{r}(\bar{u}^R_{(1)}))\bar{l}(\cdot) - \bar{a}(\cdot, \bar{u}^R_{(3)}).$$

We define, for any $\mu \in \mathcal{P}$, the coercivity factor

$$\bar{\alpha}(\mu) = \inf_{v \in \bar{X} \setminus \{0\}} \frac{\bar{a}(v, v; \mu)}{\|v\|_{\bar{X}}^2}$$

and the continuity factor

(14)
$$\bar{\gamma}_{(2)}(\mu) = \sup_{w,v \in \bar{X} \setminus \{0\}} \frac{\mathbb{E}[l(w;\mu,\cdot)l(v;\mu,\cdot)]}{\|w\|_{\bar{X}} \|v\|_{\bar{X}}}.$$

It is possible to replace these factors by efficiently computable upper and lower bounds [13]. We introduce the dual space \bar{X}' of \bar{X} with norm

(15)
$$||F||_{\bar{X}'} := \sup_{v \in \bar{X} \setminus \{0\}} \frac{|F(v)|}{||v||_{\bar{X}}} \qquad \forall F \in \bar{X}'.$$

We can derive the following error bound for the error in the reduced-order approximation of the solution:

Lemma 3.6 (solution bound). For given $\mu \in \mathcal{P}$,

(16)
$$\|\bar{u} - \bar{u}^R\|_{\bar{X}} \le \frac{\|\bar{r}\|_{\bar{X}'}}{\bar{\alpha}}.$$

Proof. Analog to the proof of Lemma 2.7.

In view of the definition of the weak linear form \bar{l} , we obtain the following bounds for the expected value and variance of the output:

Theorem 3.7 (expected output bound). For given $\mu \in \mathcal{P}$,

(17)
$$|\mathbb{E}[l(\bar{u})] - \bar{l}(\bar{u}^R) + \bar{r}(\bar{u}_{(1)}^R)| \le \frac{\|\bar{r}\|_{\bar{X}'}\|\bar{r}_{(1)}\|_{\bar{X}'}}{\bar{\alpha}}.$$

Proof. Analog to the proof of Lemma 2.8.

Theorem 3.8 (output variance bound). For given $\mu \in \mathcal{P}$,

(18)
$$\begin{aligned} \left| \mathbb{V}[l(\bar{u})] - \mathbb{V}[l(\bar{u}^R)] - \bar{r}(\bar{u}_{(1)}^R)^2 + \bar{r}(\bar{u}_{(2)}^R) - \bar{r}(\bar{u}_{(3)}^R) \right| \\ &\leq \frac{\bar{\gamma}_{(2)} \|\bar{r}\|_{\bar{X}'}^2}{\bar{\alpha}^2} + \frac{\|\bar{r}\|_{\bar{X}'}^2 \|\bar{r}_{(1)}\|_{\bar{X}'}^2}{\bar{\alpha}^2} + \frac{\|\bar{r}_{(2)} - \bar{r}_{(3)}\|_{\bar{X}'} \|\bar{r}\|_{\bar{X}'}}{\bar{\alpha}}. \end{aligned}$$

Proof. Setting $e = \bar{u} - \bar{u}^R$, we rewrite

(19)
$$\bar{r}(\bar{u}_{(2)}^R) \stackrel{(10),(9)}{=} \bar{a}(e,\bar{u}_{(2)}^R) \stackrel{(12)}{=} -2\mathbb{E}[l(\bar{u}^R)l(e)] - \bar{r}_{(2)}(e),$$

(20)
$$\bar{r}(\bar{u}_{(3)}^R) \stackrel{(10),(9)}{=} \bar{a}(e,\bar{u}_{(3)}^R) \stackrel{(13)}{=} -2(\bar{l}(\bar{u}^R) - \bar{r}(\bar{u}_{(1)}^R))\bar{l}(e) - \bar{r}_{(3)}(e).$$

After expressing the variance in terms of expectations, the left-hand side of (18) becomes

$$\begin{split} \Big| \underbrace{ \mathbb{E}[l(\bar{u})^2] - \mathbb{E}[l(\bar{u}^R)^2] + \bar{r}(\bar{u}^R_{(2)})}_{=\mathbb{E}[l(e)^2] - \bar{r}_{(2)}(e) \text{ by (19)}} \underbrace{ -\bar{l}(\bar{u})^2 + \bar{l}(\bar{u}^R)^2 - \bar{r}(\bar{u}^R_{(1)})^2 - \bar{r}(\bar{u}^R_{(3)})}_{=\bar{r}_{(3)}(e) - (\bar{l}(e) + \bar{r}(\bar{u}^R_{(1)}))^2 \text{ by (20)}} \Big| \\ \leq \Big| \mathbb{E}[l(e)^2] \Big| + (\bar{l}(e) + \bar{r}(\bar{u}^R_{(1)}))^2 + \Big| \bar{r}_{(2)}(e) - \bar{r}_{(3)}(e) \Big|. \end{split}$$

The final result follows from the following bounds:

(21)
$$|\mathbb{E}[l(e)^2]| \stackrel{(14)}{\leq} \bar{\gamma}_{(2)} ||e||_{\bar{X}}^2 \stackrel{(16)}{\leq} \frac{\bar{\gamma}_{(2)} ||\bar{r}||_{\bar{X}'}^2}{\bar{\alpha}^2},$$

$$(22) (\bar{l}(e) + \bar{r}(\bar{u}_{(1)}^{R}))^{2} \stackrel{(17)}{\leq} \frac{\|\bar{r}\|_{\bar{X}'}^{2} \|\bar{r}_{(1)}\|_{\bar{X}'}^{2}}{\bar{\alpha}^{2}}, \\ |\bar{r}_{(2)}(e) - \bar{r}_{(3)}(e)| \stackrel{(15)}{\leq} \|\bar{r}_{(2)} - \bar{r}_{(3)}\|_{\bar{X}'} \|e\|_{\bar{X}} \stackrel{(16)}{\leq} \frac{\|\bar{r}_{(2)} - \bar{r}_{(3)}\|_{\bar{X}'} \|\bar{r}\|_{\bar{X}'}}{\bar{\alpha}}.$$

4. Reduced spaces. We introduce candidate reduced spaces X^R and \bar{X}^R to be used in Problems 2.2 and 3.2, respectively. For simplicity, we focus on spaces generated by snapshot-based proper orthogonal decomposition (POD), but the theory of sections 2 and 3 does not dependent on this choice. For instance, the availability of computable error bounds also allows the use of greedy snapshot sampling [3, 11, 17].

The procedures described in this section can also be applied to create the dual reduced spaces encountered in Problems 2.5 and 3.4, by applying the POD to snapshots of the corresponding discretized dual solutions. The creation of the dual reduced spaces must follow a

certain sequence because some of the discretized dual problems contain reduced primal and dual solutions on their right-hand sides. For instance, creating $\bar{X}^R_{(3)}$ from samples of $\bar{u}_{(3)}$ requires the availability of \bar{X}^R and $\bar{X}^R_{(1)}$ due to the right-hand side of the discretized dual problem that defines $\bar{u}_{(3)}$, see Problem 3.3.

We motivate the POD spaces by corresponding continuous minimization problems. We discretize these minimization problems using quadrature [22, sections 6.4 and 6.5]. The discrete minimization problems can be solved using a weighted singular value decomposition of a snapshot matrix, based on [14]. Algorithm 1 provides a definition of the POD algorithm in terms of linear algebra, assuming N snapshot vectors of length M. The algorithm is formulated in a way that allows a general snapshot weighting and the maximum possible number of output vectors. Actual implementations can benefit from using a simpler (diagonal) snapshot weighting matrix and assuming a small number of output vectors. Subsections 4.1 and 4.2 describe how to generate the input to the algorithm in order to compute POD basis vectors from available FE or SGFE snapshots.

Algorithm 1 Proper orthogonal decomposition.

Input: Snapshot matrix $\mathcal{U} = (U^1, \dots, U^N) \in \mathbb{R}^{M \times N}$. Symmetric positive definite weighting matrices $S \in \mathbb{R}^{M \times M}$ and $W \in \mathbb{R}^{N \times N}$.

Output: POD basis matrix $\Phi = (\Phi_1, \dots, \Phi_M) \in \mathbb{R}^{M \times M}$.

- 1: Compute Cholesky factor \tilde{S} such that $S = \tilde{S}^T \tilde{S}$.
- 2: Compute Cholesky factor $\tilde{\mathcal{W}}$ such that $\mathcal{W} = \tilde{\mathcal{W}}^T \tilde{\mathcal{W}}$.
- 3: Compute singular value decomposition $\tilde{\Phi}\Sigma\tilde{\mathcal{V}}^T$ of $\tilde{\mathcal{S}}\mathcal{U}\tilde{\mathcal{W}}^T$.
- 4: Solve $\tilde{S}\Phi = \tilde{\Phi}$ for Φ .

4.1. Spatial POD. We provide a POD of snapshots of the solution u of Problem 2.1, resulting in a spatial POD space $X^R = \operatorname{span}(\varphi_1, \ldots, \varphi_R)$ for $R \leq M_{\text{FE}}$. One can define a POD basis as a set of functions which solve the continuous minimization problems

(23)
$$\min_{\varphi_1, \dots, \varphi_R \in X} \int_{\mathcal{P}} \int_{\Xi} \left\| u(y, \mu) - \sum_{r=1}^R (u(y, \mu), \varphi_r)_X \varphi_r \right\|_{X}^2 d\mathbb{P}_{\xi}(y) d\mu, \quad (\varphi_i, \varphi_j)_X = \delta_{ij},$$

for $R = 1, ..., M_{\text{FE}}$. We approximate the double integral using Monte Carlo quadrature.

Concerning the Monte Carlo quadrature of the Ξ -integral on the one hand, we already know that the reduced-order model will only be evaluated at the random parameter points y^1, \ldots, y^{N_ξ} , because the Monte Carlo discretization of the final stochastic estimates is fixed from the beginning. We use exactly these points for the discretization of the POD minimization problem, too, because with this choice our reduced basis will be optimal in a mean-square sense with respect to approximating the finite element solution at y^1, \ldots, y^{N_ξ} .

Concerning the Monte Carlo quadrature of the \mathcal{P} -integral on the other hand, our model should be able to estimate the output statistics reasonably well at any point in \mathcal{P} . Having no further information about how the reduced-order model will ultimately be used, we discretize the deterministic parameter domain using a training set $\mathcal{P}^{N_{\mu}^{\text{train}}} = \{\mu^1, \dots, \mu^{N_{\mu}^{\text{train}}}\}$, with $\mu^1, \dots, \mu^{N_{\mu}^{\text{train}}}$ distributed independently and uniformly over \mathcal{P} . When testing the performance

of the resulting reduced-order model, we use a different set of points in the parameter domain in order to verify the robustness of the model with respect to the deterministic parameter.

The Monte Carlo quadrature of the double integral in (23) finally results in a set of discretized POD minimization problems

(24)
$$\min_{\varphi_1, \dots, \varphi_R \in X} \frac{1}{N_{\xi} N_{\mu}^{\text{train}}} \sum_{i=1}^{N_{\xi}} \sum_{j=1}^{N_{\mu}^{\text{train}}} \left\| u(y^i, \mu^j) - \sum_{r=1}^{R} (u(y^i, \mu^j), \varphi_r)_X \varphi_r \right\|_{X}^{2}, \quad (\varphi_i, \varphi_j)_X = \delta_{ij},$$

for $R=1,\ldots,M_{\rm FE}$. For the POD computation in terms of Algorithm 1, we set $N=N_{\xi}N_{\mu}^{\rm train}$ and $M=M_{\rm FE}$ and let $U^{(i-1)N_{\xi}+j}\in\mathbb{R}^M$ be the coefficient vector corresponding to the expansion of $u(y^i,\mu^j)\in X$ in a basis of X for $i=1,\ldots,N_{\xi}$ and $j=1,\ldots,N_{\mu}^{\rm train}$. By substituting the finite element basis expansions into (24), we find

$$\mathcal{S} = \mathcal{M}_X, \quad \mathcal{U} = (U^1, \dots, U^N), \quad \mathcal{W} = \frac{1}{N} I_N,$$

where \mathcal{M}_X denotes the mass matrix corresponding to X and I_N denotes the $N \times N$ identity matrix. The output of Algorithm 1 is a POD basis matrix $\Phi = (\Phi_1, \dots, \Phi_{M_{\text{FE}}}) \in \mathbb{R}^{M_{\text{FE}} \times M_{\text{FE}}}$. The i-th POD basis function φ_i can be obtained from the i-th POD basis vector Φ_i via an expansion in the available basis of X, using the elements of Φ_i as expansion coefficients. Finally, an R-dimensional POD reduced space is given by $X^R = \text{span}(\varphi_1, \dots, \varphi_R)$ for any $R = 1, \dots, M_{\text{FE}}$ and the trivial space $X^0 \subset X$ contains only the zero function.

4.2. Spatial-stochastic POD. We introduce a reduced basis space that can be used to derive a stochastic Galerkin reduced basis method. It employs a simultaneous reduction of the spatial and stochastic degrees of freedom of a stochastic Galerkin finite element discretization.

Spatial-stochastic POD reduced basis functions can be defined as solutions to a set of \mathcal{P} -continuous POD minimization problems

$$\min_{\bar{\varphi}_1, \dots, \bar{\varphi}_R \in \bar{X}} \int_{\mathcal{P}} \left\| \bar{u}(\mu) - \sum_{r=1}^R (\bar{u}(\mu), \bar{\varphi}_r)_{\bar{X}} \bar{\varphi}_r \right\|_{\bar{X}}^2 d\mu, \quad (\bar{\varphi}_i, \bar{\varphi}_j)_{\bar{X}} = \delta_{ij},$$

for $R=1,\ldots,M_{\rm FE}M_{\rm SG}$. A Monte Carlo quadrature of the \mathcal{P} -integral raises the issue of choosing the sample points. Using the same training set $\mathcal{P}^{N_{\mu}^{\rm train}}=\{\mu^1,\ldots,\mu^{N_{\mu}^{\rm train}}\}$ as in subsection 4.1 leads to discrete POD minimization problems

(25)
$$\min_{\bar{\varphi}_1, \dots, \bar{\varphi}_R \in \bar{X}} \frac{1}{N_{\mu}^{\text{train}}} \sum_{n=1}^{N_{\mu}^{\text{train}}} \left\| \bar{u}(\mu^n) - \sum_{r=1}^{R} (\bar{u}(\mu^n), \bar{\varphi}_r)_{\bar{X}} \bar{\varphi}_r \right\|_{\bar{X}}^2, \quad (\bar{\varphi}_i, \bar{\varphi}_j)_{\bar{X}} = \delta_{ij}$$

for $R = 1, ..., M_{\text{FE}}M_{\text{SG}}$. Regarding the POD computation in terms of Algorithm 1, we set $N = N_{\mu}^{\text{train}}$ and $M = M_{\text{FE}}M_{\text{SG}}$ and denote the stochastic Galerkin finite element coefficient vector of $\bar{u}(\mu^n)$ by U^n . By substituting the stochastic Galerkin finite element basis expansions into (25), we obtain

$$\mathcal{S} = \mathcal{M}_S \otimes \mathcal{M}_X, \quad \mathcal{U} = \left(U^1, \dots, U^{N_\mu^{\mathrm{train}}}\right), \quad \mathcal{W} = \frac{1}{N_\mu^{\mathrm{train}}} I_{N_\mu^{\mathrm{train}}},$$

where $I_{N_{\mu}^{\text{train}}}$ is the $N_{\mu}^{\text{train}} \times N_{\mu}^{\text{train}}$ identity matrix and \mathcal{M}_S is the mass matrix containing the mutual S-inner products of the basis functions used to represent S. In view of Algorithm 1, the i-th POD basis function $\bar{\varphi}_i$ can be obtained from the i-th POD basis vector Φ_i via an expansion in the available basis of \bar{X} , using the elements of Φ_i as expansion coefficients. Finally, an R-dimensional POD reduced space is given by $\bar{X}^R = \text{span}(\bar{\varphi}_1, \dots, \bar{\varphi}_R)$ for any $R = 1, \dots, M_{\text{FE}}M_{\text{SG}}$ and the trivial space $\bar{X}^0 \subset \bar{X}$ contains only the zero function.

- **5. Numerical experiments.** We assess the provided error bounds and compare the accuracy of the MCRB and SGRB models in terms of computing the expectation and variance of a linear output for a convection-diffusion-reaction problem.
- **5.1. Example problem.** Let $y=(y_1,\ldots,y_K)^T\in\Xi\subset\mathbb{R}^K$ denote the value of a sample of a random parameter vector, $\mu=(\mu_1,\mu_2)^T\in\mathcal{P}\subset\mathbb{R}^2$ the value of a deterministic parameter vector and $x=(x_1,x_2)^T\in\Omega\subset\mathbb{R}^2$ the coordinate in the computational domain Ω . We model the random input by a second-order random field with expected value κ_0 and separable exponential covariance $c(x)=\sigma^2\exp(-|x_1|/L-|x_2|/L)$, where σ is the standard deviation and L is the correlation length. We approximate the random field using a truncated Karhunen-Loève expansion $\kappa(x;y)=\kappa_0+\sigma\sum_{k=1}^K\sqrt{\lambda_k}\kappa_k(x)y_k$, where λ_k denote the eigenvalues of the corresponding eigenvalue problem, ordered decreasingly by magnitude, and $\kappa_k(x)$ denote respective eigenfunctions. The covariance function allows for an analytical solution of the eigenvalue problem [9]. We assume that the parameters of the Karhunen-Loève expansion originate from independent uniformly distributed random variables. The truncation index K can be interpreted as a modeling parameter, because it enters the definition of the bilinear form. The governing equations of our example problem are provided as follows:

Problem 5.1 (spatial strong form). For any $(y,\mu) \in \Xi \times \mathcal{P}$, find $u(\cdot;y,\mu) \colon \Omega \to \mathbb{R}$ such that

$$\mu \cdot \nabla u(x; y, \mu) - \Delta u(x; y, \mu) - \kappa(x; y)u(x; y, \mu) = 1, \quad x \in \Omega,$$
$$u(x; y, \mu) = 0, \quad x \in \partial \Omega.$$

The deterministic parameter vector $\mu \in \mathcal{P} \subset \mathbb{R}^2$ can be interpreted as a spatially uniform convective velocity. The random parameter vector $y \in \Xi \subset \mathbb{R}^K$ enters via a parametrized random reactivity. A concrete instance of the example problem is determined by the model parameters given in Table 1. The output of the example problem is given by $l(u(y,\mu);y,\mu)$, where

(26)
$$l(v; y, \mu) = \int_0^{\frac{1}{2}} \int_0^{\frac{1}{2}} v(x) \, \mathrm{d}x_1 \, \mathrm{d}x_2.$$

In order to express the example problem in terms of the spatial weak form of Problem 2.1, we set

(27)
$$a(w, v; y, \mu) = a^{0}(w, v) + \sum_{k=1}^{K} y_{k} a_{y}^{k}(w, v) + \sum_{p=1}^{2} \mu_{p} a_{\mu}^{p}(w, v),$$

symbol	value	description
κ_0	-1000	expected value of reactivity
σ	200	standard deviation of reactivity
L	1	correlation length
K	5	Karhunen-Loève truncation index
Ω	$(-0.5, 0.5)^2$	spatial domain with boundary $\partial\Omega$
${\cal P}$	$[-200, 200]^2$	deterministic parameter domain
Ξ	$[-\sqrt{3},\sqrt{3}]^K$	random parameter domain

Table 1 *Model parameters of the test problem.*

with

$$a^{0}(w,v) = \int_{\Omega} \nabla w(x) \cdot \nabla v(x) \, dx - \kappa_{0} \int_{\Omega} w(x)v(x) \, dx,$$

$$a_{y}^{k}(w,v) = \sigma \sqrt{\lambda_{k}} \int_{\Omega} \kappa_{k}(x)w(x)v(x) \, dx, \qquad k = 1, \dots, K,$$

$$a_{\mu}^{p}(w,v) = \int_{\Omega} \partial_{x_{p}} w(x)v(x) \, dx, \qquad p = 1, 2$$

and

(28)
$$f(v; y, \mu) = \int_{\Omega} v(x) \, \mathrm{d}x.$$

A spatial weak form of Problem 5.1 is provided in terms of the standard infinite-dimensional Sobolev space $H_0^1(\Omega)$ as follows:

Problem 5.2 (spatial weak form). For given $(y, \mu) \in \Xi \times \mathcal{P}$, find

$$u(y,\mu) \in H_0^1(\Omega) : \quad a(u(y,\mu), v; y, \mu) = f(v; y, \mu) \quad \forall v \in H_0^1(\Omega).$$

By taking the expectation and using the notation of subsection 3.1, a spatial-stochastic weak form is given by

Problem 5.3 (spatial-stochastic weak form). For given $\mu \in \mathcal{P}$, find

$$\bar{u}(\mu) \in L^2_{\mathcal{E}}(\Xi, H^1_0(\Omega)) : \quad \bar{a}(\bar{u}(\mu), v; \mu) = \bar{f}(v; \mu) \quad \forall v \in L^2_{\mathcal{E}}(\Xi, H^1_0(\Omega)).$$

5.2. Discretization. The MCFE and SGFE discretizations (Problems 2.1 and 3.1) provide necessary links between the infinite-dimensional test problems (Problems 5.2 and 5.3) and the respective reduced-order models (Problems 2.2 and 3.2). In the following, we describe the computational details of the MCFE and SGFE discretizations of the test problem. Table 2 lists our choice of the relevant discretization parameters.

Table 2
Discretization parameters of the test problem. The default values are used in the snapshot simulations.
The reference values are used to assess the accuracy of the snapshot discretizations.

symbol	default	reference	description
$M_{ m FE}$	225	961	number of FE degrees of freedom
N_{ξ}	1024	16384	number of MC samples of $y \in \Xi$
d	2	3	degree of SG polynomials
$M_{ m SG}$	243	1024	number of SG degrees of freedom: $(d+1)^K$

Finite element method. We derive an instance of the stochastic strong finite element problem by replacing $H_0^1(\Omega)$ in Problem 5.2 with a finite-dimensional subspace. In particular, we employ the space $X \subset H_0^1(\Omega)$ formed by continuous piecewise linear finite elements corresponding to a regular graded simplicial triangulation of Ω , characterized by the number $M_{\rm FE}$ of finite element degrees of freedom. We estimate the spatial discretization error using simulations on a finer reference triangulation as a substitute for the exact solution.

Monte Carlo method. We provide estimates of the expectation and variance by discretizing the respective stochastic integrals using Monte Carlo quadrature in the sense of subsection 2.1. To this end, we generate random samples $y^1, \ldots, y^{N_\xi} \in \Xi$ according to the distribution \mathbb{P}_ξ with a standard pseudorandom number generator. A reference simulation with a higher number of samples delivers an estimate of the sampling error.

Stochastic Galerkin method. Stochastic Galerkin methods estimate the expectation and variance by directly evaluating the respective stochastic integrals, given a stochastic Galerkin solution based on a finite-dimensional subspace of $L^2_{\varepsilon}(\Xi)$. In general, a stochastic Galerkin finite element method applied to a linear elliptic problem with a random elliptic coefficient leads to a large, block-structured system of linear algebraic equations. In our case, however, the underlying random variables y_1, \ldots, y_K are independent and enter the bilinear form linearly, see (27). Under these conditions, it is possible to find a double-orthogonal polynomial basis which decouples the blocks in the system matrix [1, 7]. The resulting block-diagonal system of equations can be solved efficiently due to the relatively small bandwidth and the ability to treat the blocks in parallel. To define a suitable double-orthogonal basis, we start with K spaces of possibly different dimensions, spanned by univariate Legendre polynomials over the interval $[-\sqrt{3}, \sqrt{3}]$. We normalize the polynomials regarding the underlying uniform distribution and rotate the bases such that they consist of double-orthogonal univariate polynomials, as described in [1]. Finally, a tensor product of these univariate double-orthogonal polynomial bases forms a basis of an $M_{\rm SG}$ -dimensional subspace $S\subset L^2_\xi(\Xi)$. In our experiments, we use the same polynomial degree d in all directions. We assess the error associated with the choice of d by comparing with a reference solution using a higher degree.

Reduced basis. The considered reduced-order models rely on POD spaces generated from snapshots of the underlying discretized solution. We choose $N_{\mu}^{\rm train}=64$ as the number of training samples in the deterministic parameter domain. Consequently, section 4 specifies the creation of the reduced spaces.

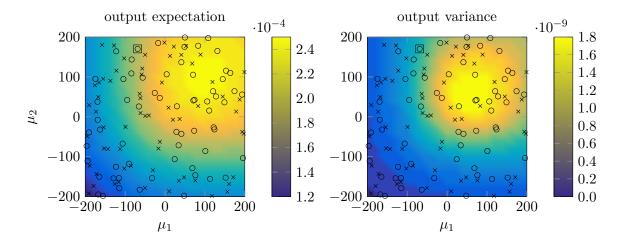


Figure 1. Parameter-dependent output expectation $\mathbb{E}[l(u(\cdot,\mu);\cdot,\mu)]$ and variance $\mathbb{V}[l(u(\cdot,\mu);\cdot,\mu)]$ for the functional l given by (26). Crosses mark the snapshot parameter values. The square marks the parameter value corresponding to Figure 2. Circles mark the parameter values used to obtain Figure 3.

5.3. Results. Figure 1 presents the parameter-dependent output statistics obtained with the default parameter-dependent SGFE model. The crosses in Figure 1 correspond to the snapshot training parameter values provided by the pseudo random number generator. Additionally, Figure 1 shows the test parameter values that are used to assess the model.

The reduced basis estimates of the output statistics together with the respective error bounds are provided by Theorems 2.9 and 2.10 for the MCRB method and Theorems 3.7 and 3.8 for the SGRB method. First, we validate the error bounds for a single random realization of the deterministic parameter, marked by a square in Figure 1. The convergence regarding the number of reduced basis functions R is presented in Figure 2. The error components of the underlying discretized solution are provided as a reference. Looking at the discretization errors only, we see that number of MC samples is sufficient to approximate the expectation but actually too small to balance the FE error in case of the variance. The SG error, on the other hand, is smaller than the FE error in all cases, which provides evidence that the stochastic Galerkin discretization of the stochastic domain is sufficiently fine. Concerning the reduced basis models, we observe that $R \approx 16$ reduced basis functions are sufficient to obtain reduced-order estimates which are on a par with the full-order estimates in all considered cases. The plots suggest that all error bounds converge at the same rates as the respective errors. This is useful, because it implies that efficiency of the error bounds does not become significantly worse when the number of reduced basis functions is increased.

We assess the convergence globally over \mathcal{P} in order to confirm that the point-wise observation in the deterministic parameter space provided by Figure 2 is not a lucky coincidence. To this end, we employ an $L^2(\mathcal{P})$ -norm, approximated using Monte Carlo quadrature with $N_{\mu}^{\text{test}} = 64$ samples shown as circles in Figure 1. The convergence results are presented in Figure 3. Since we have averaged over the parameter space, the plots appear less random than the plots in Figure 2. The convergence of the estimates and the corresponding bounds correspond quite well. Moreover, the MCRB and SGRB methods perform similar in terms of

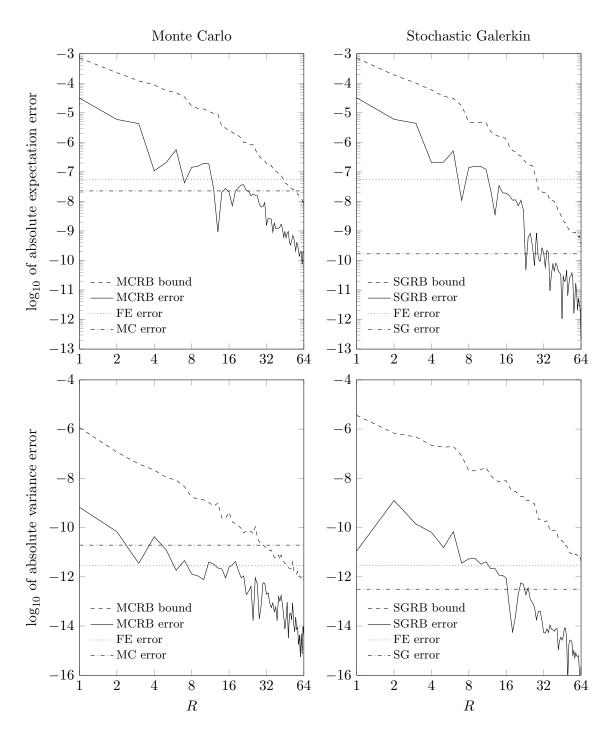


Figure 2. Log-log plots of the errors in the approximation of the expectation (top row) and variance (bottom row) of a linear functional with an MCRB method (left column) and an SGRB method (right column) depending on the dimension R of the reduced spaces, for a random point in the deterministic parameter domain. Respective error bounds and approximate FE/SG/MC discretization errors.

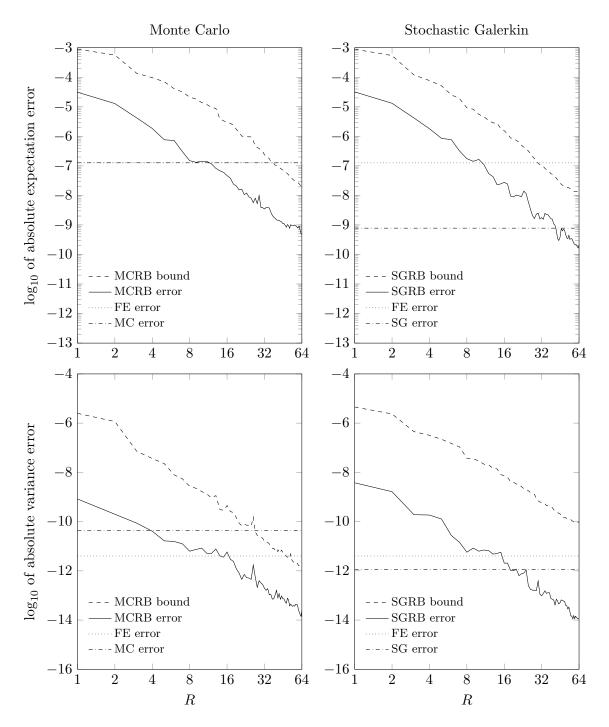


Figure 3. Log-log plots of the errors in the approximation of the expectation (top row) and variance (bottom row) of a linear functional with an MCRB method (left column) and an SGRB method (right column) depending on the dimension R of the reduced spaces, measured in terms of an approximate $L^2(\mathcal{P})$ -norm. Respective error bounds and approximate FE/SG/MC discretization errors. It is a coincidence that the approximate FE and MC errors of the estimated expectation are very close in this outcome of the random experiment.

accuracy per number of basis functions.

In Figures 2 and 3, it appears that the SGRB error bound over-estimates the actual error more severely (by 4 orders of magnitude) than the MCRB error bound (2 orders of magnitude). A closer inspection of the individual components of the error estimate reveals that for larger R the lower-order term involving the continuity factor becomes responsible for the major portion of the error estimate. In particular, for R=64 at the parameter point corresponding to Figure 2, the terms on the right-hand side of Theorem 3.8 amount to approximately $4.2 \cdot 10^{-12}$, $1.2 \cdot 10^{-19}$ and $5.2 \cdot 10^{-14}$, respectively.

6. Conclusion. We have observed that the SGRB method can deliver estimates of the expectation and variance of linear outputs with an accuracy similar to the MCRB method. Also, the SGRB error bounds regarding the expected value were very close to the respective MCRB bounds in our experiments. Concerning the variance, the presented SGRB bounds overestimate the error more severely than the available MCRB bounds, which opens opportunities for future improvement of the SGRB variance bound. Nevertheless, the MCRB and SGRB variance bounds both converge at the same order depending on the number of reduced basis functions. This behavior is reflected by the theory, which predicts the same order of convergence in terms of dual norms of residuals.

The MCRB statistical output estimates and error bounds require a Monte Carlo sampling of the reduced quantities point-wise in the random parameter domain. In our tests, 1024 samples were sufficient to balance the finite element error for the expectation, but an accurate prediction of the variance would require even more samples. The SGRB estimates and bounds, on the other hand, are obtained by an exact integration of the corresponding reduced basis expansions in the setup phase of the reduced-order model, and, thus, do not rely on Monte Carlo sampling. As a consequence, the primal and dual SGRB problems need to be solved only once for each new deterministic parameter. In our tests, the SGRB and the MCRB methods achieved a similar reduction of degrees of freedom for given error tolerance. As a consequence, the possible speedup of SGRB methods compared to MCRB methods is in the order of magnitude of the number of Monte Carlo samples.

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