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Karhunen-Loève Expansion

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Preprint Series: 2012 - 05



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REDUCED BASIS METHODS FOR PARAMETERIZED PARTIAL DIFFERENTIAL EQUATIONS WITH STOCHASTIC INFLUENCES USING THE KARHUNEN-LOÈVE EXPANSION

BERNARD HAASDONK, KARSTEN URBAN, AND BERNHARD WIELAND*

ABSTRACT. We consider parametric partial differential equations (PPDEs) with stochastic influences e.g. in terms of random coefficients. Using standard discretizations such as finite elements, this often amounts to high-dimensional problems. In a multi-query context, the PPDE has to be solved for various instances of the deterministic parameter as well as the stochastic influences. To decrease computational complexity, we derive a reduced basis (RB) method, where the uncertainty in the coefficients is modeled using Karhunen-Loève (KL) expansions. We restrict ourselves to linear coercive problems with linear and quadratic output functionals. A new *a-posteriori* error analysis is presented that generalizes and extends some of the results by Boyaval et al. [3]. The additional KL-truncation error is analyzed for the state, output functionals and also for statistical outputs such as mean and variance. Error estimates for quadratic outputs are obtained using additional non-standard dual problems. Numerical experiments for a two-dimensional porous medium demonstrate the effectivity of this approach.

1. INTRODUCTION

Several problems in science, medicine, economy and engineering are modeled by partial differential equations (PDE) with stochastic influences. One could think of measurements that are uncertain or unknown spatial coefficients such as porosity. Examples include porous media flows (e.g. groundwater, Li-ion batteries or fuel cells), models in finance or inverse problems. In addition to such uncertainties, many problems also depend on a number of (deterministic) parameters, i.e., one has a parameterized PDE (PPDE). Examples include geometry, model parameters or forces. We are particularly interested in situations where the PPDE with stochastic influences has to be evaluated quite often for various instances of the deterministic parameters and the stochastic influences. In the stochastic framework, such a situation occurs e.g. in Monte Carlo simulations to compute statistical quantities such as mean, variance or other moments. For the deterministic parameters, one might think of parameter studies or optimization. Such a multi-query situation requires the numerical solution of the PDE for many instances of parameter and

Date: April 20, 2012.

2010 Mathematics Subject Classification. 35R60, 65M15, 65M60.

Key words and phrases. Reduced Basis Methods, Stochastic Partial Differential Equations, Karhunen-Loève Decomposition, Error Estimators.

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K.U. has been supported by the Deutsche Forschungsgemeinschaft (DFG) under GrK 1100 and Ur-63/9. B.W. is funded by the state of Baden-Württemberg within the Landesgraduierten program. This paper was partly written while K.U. was Visiting Professor at MIT, Cambridge (USA). The authors thank Sébastien Boyaval for fruitful discussions on the topic of the paper.

stochastic influence which is infeasible in particular for more complex PDEs. Hence, model reduction is required.

It should be noted that we are *not* concerned with stochastic PDEs involving the Itô calculus. This is the reason why we use the term *PDEs with stochastic influences*, even though this might be a bit lengthy.

The reduced basis method (RBM) has intensively been studied for the numerical solution of PPDEs, e.g. [7, 15, 16, 19], a complete list of references would go far beyond the scope of this paper. The basic idea is an offline-online decomposition combined with a rigorous a-posteriori error control. In the offline stage, a reduced basis is formed by solving the complex PPDE for certain parameter values, so-called snapshots. The selection is based upon a Greedy algorithm using a rigorous error bound, [20]. The so formed reduced system is then used in the online stage for a highly efficient simulation for a given new parameter.

One might think that this approach can immediately be used also for PPDEs with stochastic influences, viewing the stochasticity, i.e. stochastic events or inputs, as additional parameters. However, unlike for deterministic parameters, we have generally no distance measure in the probability space at our disposal, so that the ideas cannot be transferred directly. A basic assumption of the RBM is a smooth dependence of the solution of the PPDE w.r.t. the parameter, which can not be assured due to the lack of the distance measure. Furthermore, the dimension of the parameter space crucially influences the efficiency of the RBM. In the case of stochastic influences, the parameter space may be infinite-dimensional.

As a way-out, we propose to use a Karhunen-Loève (KL) expansion [12, 13, 17] of the stochastic process and appropriately truncate it. Even though the resulting expansion coefficients are still random variables, i.e. functions w.r.t. the stochastic event, we treat them in some way as parameters that can be modeled using polynomial chaos (PC) expansions [21, 22]. The KL truncation error of course has to be analyzed. The KL expansion shows some resemblance to the empirical interpolation method (EIM) [2, 18] in order to obtain an affine decomposition of random and spatial variables, where the random variables correspond to the parameter dependent EIM coefficients. Consequently, our analysis is in some parts similar to the EIM analysis e.g. in [18].

PDEs with stochastic influences have been widely studied in the literature, where, apart from Monte Carlo methods, also weak solutions in space *and* probability are considered. These techniques are also known as stochastic collocation methods [1] or stochastic finite elements [6]. For more information we refer to [5, 8, 14] and the references therein.

So far, not much work on RBM regarding stochastic problems has been done. In [3], Boyaval et al. studied a specific problem with stochastic Robin-type boundary conditions. However, to the best of our knowledge, the analysis presented there does not cover the case of general stochastic influences, e.g. in terms of random spatial coefficients. In this sense, the present paper generalizes and extends the findings in [3]. For the sake of completeness, let us also mention [4], where an RB control variate technique for variance reduction is introduced.

In particular in the presence of stochastic influences, one is not only interested in a good approximation of the state, i.e. the solution of the PPDE, but in accurate outputs, together with corresponding statistical quantities such as expectation or variance. The latter requires the computation of quadratic output functionals.

Different RBMs for quadratic outputs have been studied. These methods use expanded formulations that eliminate the nonlinearity [9], or introduce special dual problems [10]. Due to the KL truncation effects, however, these approaches cannot be used directly for our problem at hand. Hence, we introduce two more modified dual linear problems in order to derive a-posteriori error bounds also for the above mentioned statistical quantities. These error estimates can then be used in a standard Greedy approach [20] for the offline snapshot selection.

We are aware of the fact that the stochastic influences in general cause the underlying problem to be high-dimensional. This leads to the necessity of solving high-dimensional problems in the offline stage which calls for the use of specific numerical methods. This aspect, however, is not investigated in this paper, also since we consider a Monte Carlo framework w.r.t. the stochasticity.

The remainder of the paper is organized as follows. In Section 2, we collect known facts on variational problems with stochastic influences, the KL expansion and the RBM. We restrict ourselves to linear coercive problems. Section 3 contains our a-posteriori error analysis for the primal and dual solution as well as linear and quadratic outputs. In Section 4, we introduce the error analysis for the statistical quantities such as moments and variances. Note that since the operator has stochastic influences, we cannot derive a deterministic PDE for linear moments such as the expectation even for linear PDEs. The offline-online decomposition is presented in Section 5 as well as a method to compute coercivity lower bounds adjusted to stochastic problems. Our numerical experiments are described in Section 6.

2. PRELIMINARIES

In this section, we collect the basic features of the problem under consideration.

2.1. Variational problems with stochastic influences. Let $D \subset \mathbb{R}^d$ be an open, bounded domain, $\mathcal{D} \subset \mathbb{R}^P$ a set of deterministic parameters and $(\Omega, \mathfrak{A}, \mathbb{P})$ a probability space. For some $X \subset H^1(D)$ (accounting also for the corresponding boundary conditions) let $a : X \times X \times \mathcal{M} \rightarrow \mathbb{R}$, $\mathcal{M} := \mathcal{D} \times \Omega$, be a possibly nonsymmetric form that is bilinear, continuous and coercive w.r.t. the first two arguments and let $f : X \times \mathcal{M} \rightarrow \mathbb{R}$ be a form with $f(\cdot; \mu, \omega) \in H^{-1}(D)$, $(\mu, \omega) \in \mathcal{M}$ such that the variational problem

$$(2.1) \quad a(u, v; \mu, \omega) = f(v; \mu, \omega), \quad v \in X,$$

admits a unique solution $u(\mu, \omega) = u(\cdot; \mu, \omega) \in X$ for all $(\mu, \omega) \in \mathcal{M}$. As an example, think of a linear elliptic second order PDE whose coefficients and right-hand side depend on deterministic parameters $\mu \in \mathcal{D}$ and stochastic inputs $\omega \in \Omega$. In particular we have the case in mind in which a coefficient function on D depends on stochastic influences modeled by ω . A formulation of type (2.1) is also called D -weak/ Ω -strong, [3], and the difference to a variational approach w.r.t. both terms, e.g. stochastic Galerkin methods [14], should be noted. As already mentioned in the introduction, the direct view of ω as an additional parameter is not entirely possible. One should think of it merely as an uncertainty, i.e., $a(\cdot, \cdot; \cdot, \omega)$ is a random variable or a stochastic process. Nevertheless, we sometimes refer to ω as the stochastic parameter.

In order to achieve computational efficiency of a RBM for (2.1), we assume both terms in (2.1) to allow for an affine decomposition with respect to the deterministic

parameter μ , namely

$$(2.2) \quad a(w, v; \mu, \omega) = \sum_{q=1}^{Q^a} \theta_q^a(\mu) [\bar{a}_q(w, v) + a_q(w, v; \omega)],$$

$$(2.3) \quad f(v; \mu, \omega) = \sum_{q=1}^{Q^f} \theta_q^f(\mu) [\bar{f}_q(v) + f_q(v; \omega)],$$

with $Q^a, Q^f \geq 1$, $\theta_q^a, \theta_q^f : \mathcal{D} \rightarrow \mathbb{R}$, $\bar{a}_q, a_q(\cdot, \cdot; \omega) : X \times X \rightarrow \mathbb{R}$ as well as $\bar{f}_q, f_q(\cdot; \omega) : X \rightarrow \mathbb{R}$ bounded for all $\omega \in \Omega$. Note that \bar{a}_q and \bar{f}_q denote the expectations of the terms in brackets, $a_q(\cdot, \cdot; \omega)$ and $f_q(\cdot; \omega)$ denote the respective fluctuating parts. In general, we do not require any further assumption on these terms. However, in Section 5, some restrictions are introduced in order to use an alternative method for the computation of coercivity lower bounds. A standard tool to derive an affine approximation of a non-affine function is the *Empirical Interpolation Method* (EIM, [2]), which, however, may not be applicable here since we have different types of parameters and influences, respectively.

In order to describe the well-posedness of (2.1), one usually defines the coercivity and continuity constants, respectively

$$(2.4) \quad \alpha(\mu, \omega) := \inf_{v \in X} \frac{a(v, v; \mu, \omega)}{\|v\|_X^2}, \quad \gamma(\mu, \omega) := \sup_{w \in X} \sup_{v \in X} \frac{a(w, v; \mu, \omega)}{\|w\|_X \|v\|_X}.$$

We assume that for some $0 < \alpha_0, \gamma_\infty < \infty$, we have

$$(2.5a) \quad \alpha(\mu, \omega) \geq \alpha_0 > 0, \quad (\text{uniform coercivity}),$$

$$(2.5b) \quad \gamma(\mu, \omega) \leq \gamma_\infty < \infty, \quad (\text{uniform continuity}),$$

for all $(\mu, \omega) \in \mathcal{D} \times \Omega$. Under these assumptions, the Lax-Milgram theorem guarantees the well-posedness of (2.1). Next, we define parameter-dependent bilinear forms and energy norms as $(\mu \in \mathcal{D}, \omega \in \Omega)$

$$(2.6) \quad (w, v)_{\mu, \omega} := a(w, v; \mu, \omega), \quad \|w\|_{\mu, \omega}^2 := (w, w)_{\mu, \omega}, \quad v, w \in X.$$

In many situations, one is not (or not only) interested in the state $u(\mu, \omega)$ or the error in the energy norm, but in some quantity of interest in terms of a linear continuous functional $\ell : X \times \mathcal{M} \rightarrow \mathbb{R}$. Again, we assume that ℓ is affine, i.e.,

$$(2.7) \quad \ell(v; \mu, \omega) = \sum_{q=1}^{Q^\ell} \theta_q^\ell(\mu) [\bar{\ell}_q(v) + \ell_q(v; \omega)]$$

with $Q^\ell \geq 1$, $\theta_q^\ell : \mathcal{D} \rightarrow \mathbb{R}$ and $\bar{\ell}_q, \ell_q(\cdot; \omega) : X \rightarrow \mathbb{R}$ bounded and linear for all $\omega \in \Omega$. If ℓ is deterministic, we set $\ell_q \equiv 0$. The output $s : \mathcal{M} \rightarrow \mathbb{R}$ is given as

$$(2.8) \quad s(\mu, \omega) := \ell(u(\mu, \omega); \mu, \omega).$$

If $\ell = f$, the output coincides with the right-hand side which is called the *compliant case*. In the non-compliant case, it is fairly standard to consider a *dual problem* of finding $p^{(1)} = p^{(1)}(\mu, \omega)$ such that for given $(\mu, \omega) \in \mathcal{D} \times \Omega$ one has

$$(2.9) \quad a(v, p^{(1)}; \mu, \omega) = -\ell(v; \mu, \omega), \quad v \in X.$$

The superscript ⁽¹⁾ in (2.9) is motivated by the fact that we will introduce further dual problems later on.

2.2. Karhunen-Loève expansion. As already stated in the introduction, we consider the well-known *Karhunen-Loève (KL) expansion* [12, 13]. Let us briefly recall the main facts. Let $\kappa : D \times \Omega \rightarrow \mathbb{R}$ be a spatial stochastic process with zero mean and existing covariance operator $\text{Cov}_\kappa(x, y) := \mathbb{E}[\kappa(x; \cdot) \kappa(y; \cdot)]$, $x, y \in D$. Let $(\lambda_k, \kappa_k(x))$, $k = 1, \dots, \infty$, be the eigenvalue/eigenfunction-pairs of the covariance operator, then the KL expansion reads

$$(2.10) \quad \kappa(x; \omega) = \sum_{k=1}^{\infty} \sqrt{\lambda_k} \xi_k(\omega) \kappa_k(x),$$

where $\xi_k : \Omega \rightarrow \mathbb{R}$ are uncorrelated random variables with zero mean and variance 1. The eigenvalues are ordered $\lambda_1 \geq \lambda_2 \geq \dots \geq 0$ and typically decay exponentially fast. One of the main reasons why we consider the KL expansion is now obvious since the above equation allows for a separation of the stochastic and the spatial terms. This is very similar to an affine expansion of a form with respect to a deterministic parameter as common in RBM. Here, we can use the deterministic, purely space-dependent terms for calculations in the offline phase so that the stochastic influences only enter through the coefficients in the KL expansion and are thus scalar quantities.

Since the KL expansion requires zero-mean random variables, the affine decompositions in (2.2), (2.3) and (2.7) are made by a separation into the deterministic expectation $\bar{a}_q, \bar{f}_q, \bar{\ell}_q$ and the zero-mean stochastic parts. We apply the KL expansion to the factors a_q, f_q , and ℓ_q . For $b \in \{a, f, \ell\}$, we get (using the correct arguments of course)

$$(2.11) \quad b(\cdot; \mu, \omega) = \sum_{q=1}^{Q^b} \theta_q^b(\mu) \left[\bar{b}_q(\cdot) + \sum_{k=1}^{\infty} \xi_{q,k}^b(\omega) b_{q,k}(\cdot) \right],$$

where for notational convenience $b_{q,k}$ also contain $\sqrt{\lambda_{q,k}^b}$ from the spectral decomposition of the corresponding covariance operator.

For numerical purposes, one usually restricts the infinite sum by some $K_q^b < \infty$. It is well-known that the KL approximation is optimal in a certain sense, [12, 13]. For $b \in \{a, f, \ell\}$ we obtain the truncated forms

$$(2.12) \quad b^K(\cdot; \mu, \omega) := \sum_{q=1}^{Q^b} \theta_q^b(\mu) \left[\bar{b}_q(\cdot) + \sum_{k=1}^{K_q^b} \xi_{q,k}^b(\omega) b_{q,k}(\cdot) \right].$$

Here and in the following, an index K indicates that the expression is or is derived from a truncated form. We do not distinguish the dependencies on K_q^b , $q = 1, \dots, Q^b$, $b \in \{a, f, \ell\}$. The truncated primal and dual problem read for $(\mu, \omega) \in \mathcal{M}$

$$(2.13) \quad a^K(u_K(\mu, \omega), v; \mu, \omega) = f^K(v; \mu, \omega), \quad v \in X,$$

$$(2.14) \quad a^K(v, p_K^{(1)}(\mu, \omega); \mu, \omega) = -\ell^K(v; \mu, \omega), \quad v \in X,$$

with solutions $u_K = u_K(\mu, \omega)$ and $p_K^{(1)} = p_K^{(1)}(\mu, \omega)$, respectively.

2.3. Reduced Basis Approximation. We consider a Reduced Basis (RB)-approximation w.r.t. our parameters $(\mu, \omega) \in \mathcal{M}$. To this end, we first consider the ‘truth’ approximation of the primal and dual problem e.g. by a finite element discretization on a sufficiently fine grid. The corresponding spaces are usually again denoted by X

indicating that the ‘truth’ approximation and the exact solution are (numerically) indistinguishable. We assume that $\dim(X) = \mathcal{N}$, where \mathcal{N} is assumed to be ‘large’.

The primal and dual RB spaces are then appropriate subspaces

$$X_N \subset X, \dim(X_N) = N \ll \mathcal{N}, \quad \tilde{X}_N^{(1)} \subset X, \dim(\tilde{X}_N^{(1)}) = \tilde{N}^{(1)} \ll \mathcal{N}.$$

Here and in following, an index N indicates that the expression denotes or is based on reduced systems. We do not explicitly indicate the dependencies on the different dimensions of the reduced systems, e.g. the dimensions of X_N and $\tilde{X}_N^{(\cdot)}$ defined below may be different. We obtain a truncated primal-dual RB formulation. For $(\mu, \omega) \in \mathcal{M}$, determine $u_{N,K} = u_{N,K}(\mu, \omega) \in X_N$, $p_{N,K}^{(1)} = p_{N,K}^{(1)}(\mu, \omega) \in \tilde{X}_N^{(1)}$ such that

$$(2.15) \quad a^K(u_{N,K}, v; \mu, \omega) = f^K(v; \mu, \omega), \quad v \in X_N,$$

$$(2.16) \quad a^K(v, p_{N,K}^{(1)}; \mu, \omega) = -\ell^K(v; \mu, \omega), \quad v \in \tilde{X}_N^{(1)}.$$

We will comment later on the specific construction of X_N and $\tilde{X}_N^{(1)}$.

3. A-POSTERIORI ERROR ANALYSIS

Now, we focus on the introduction of a-posteriori error bounds for the primal and dual problem as well as for (linear and quadratic) output functionals. We will partly follow similar considerations as in [18].

3.1. Notation. We start by fixing some notation for the subsequent analysis. In many cases, where it should be clear from the setting, we will omit the parameter (μ, ω) for notational convenience. Let

$$(3.1) \quad e_{\text{RB}}(\mu, \omega) := u_K(\mu, \omega) - u_{N,K}(\mu, \omega), \quad \tilde{e}_{\text{RB}}^{(1)}(\mu, \omega) := p_K^{(1)}(\mu, \omega) - p_{N,K}^{(1)}(\mu, \omega),$$

be the primal and dual RB error, respectively, where again u_K and $p_K^{(1)}$ denote the solution of (2.13) and (2.14), respectively. The corresponding residuals read

$$(3.2a) \quad r_{\text{RB}}(v; \mu, \omega) := f^K(v; \mu, \omega) - a^K(u_{N,K}, v; \mu, \omega) = a^K(e_{\text{RB}}(\mu, \omega), v; \mu, \omega),$$

$$(3.2b) \quad \tilde{r}_{\text{RB}}^{(1)}(v; \mu, \omega) := -\ell^K(v; \mu, \omega) - a^K(v, p_{N,K}^{(1)}; \mu, \omega) = a^K(v, \tilde{e}_{\text{RB}}^{(1)}(\mu, \omega); \mu, \omega).$$

Assuming the availability of a computable lower bound $0 < \alpha_{\text{LB}}(\mu, \omega) \leq \alpha(\mu, \omega)$ of the coercivity constant, it is fairly standard to derive RB error bounds in terms of the following quantities

$$(3.3) \quad \Delta_{\text{RB}}(\mu, \omega) := \frac{1}{\alpha_{\text{LB}}} \sup_{v \in X} \frac{r_{\text{RB}}(v)}{\|v\|_X}, \quad \tilde{\Delta}_{\text{RB}}^{(1)}(\mu, \omega) := \frac{1}{\alpha_{\text{LB}}} \sup_{v \in X} \frac{\tilde{r}_{\text{RB}}^{(1)}(v)}{\|v\|_X}.$$

Following the arguments of standard RB a-posteriori error analysis [15], the terms Δ_{RB} and $\tilde{\Delta}_{\text{RB}}^{(1)}$ account for the error caused by restricting X to X_N or $\tilde{X}_N^{(1)}$ (i.e., the RB error) given the truncated KL forms in (2.13, 2.14). Next, we investigate the KL truncation error. In view of the definition of a^K , f^K and ℓ^K we see that any truncation error depends on the random variable ω and thus on the particular realization. This dependency is somehow unsatisfactory since all derived bounds would depend on a realization of a random variable. Thus, we propose to replace the random variables $\xi_{k,q}^b(\omega)$, $k > K_q^b$, $b \in \{a, f, \ell\}$, by some ω -independent quantity. If the probability density functions of the random variables have finite support or the problem that underlies the PDE restricts their variations, we can use rigorous upper bounds ξ_{UB}^b , i.e., $|\xi_{k,q}^b(\omega)| \leq \xi_{\text{UB}}^b$, $b \in \{a, f, \ell\}$ for all $\omega \in \Omega$. In many cases,

however, it is also appropriate to use quantiles, instead. For some $0 < \rho < 1$, we define ξ_{UB}^b such that $|\xi_{k,q}^b(\omega)| \leq \xi_{\text{UB}}^b$ holds with probability $1 - \rho$, where ρ should be sufficiently small to be negligible in the following analysis. Hence, we can define the error terms for the primal and dual problem as

$$(3.4a) \quad \delta_{\text{KL}}(v; \mu, \omega) := \sum_{q=1}^{Q^a} |\theta_q^a(\mu)| \sum_{k=K_q^a+1}^{\infty} \xi_{\text{UB}}^a |a_{q,k}(u_{N,K}(\mu, \omega), v)|,$$

$$(3.4b) \quad \tilde{\delta}_{\text{KL}}^{(1)}(v; \mu, \omega) := \sum_{q=1}^{Q^a} |\theta_q^a(\mu)| \sum_{k=K_q^a+1}^{\infty} \xi_{\text{UB}}^a |a_{q,k}(v, p_{N,K}^{(1)}(\mu, \omega))|,$$

as well as for the right-hand sides $b \in \{f, \ell\}$

$$(3.4c) \quad \delta_{\text{KL}}^b(v; \mu) := \sum_{q=1}^{Q^b} |\theta_q^b(\mu)| \sum_{k=K_q^b+1}^{\infty} \xi_{\text{UB}}^b |b_{q,k}(v)|.$$

Note, that δ_{KL} and $\tilde{\delta}_{\text{KL}}^{(1)}$ still depend on ω via the RB solutions $u_{N,K}$ and $p_{N,K}^{(1)}$. The right-hand side terms δ_{KL}^f and δ_{KL}^ℓ are deterministic and thus only depend on $\mu \in \mathcal{D}$. For numerical realizations, the terms in (3.4) are usually truncated at some K_{max} , where $K_q^b < K_{\text{max}} \ll \mathcal{N} < \infty$. In a similar fashion as for the RB error, we set

$$(3.5) \quad \Delta_{\text{KL}}(\mu, \omega) := \frac{1}{\alpha_{\text{LB}}} \sup_{v \in X} \frac{\delta_{\text{KL}}(v)}{\|v\|_X}, \quad \tilde{\Delta}_{\text{KL}}^{(1)}(\mu, \omega) := \frac{1}{\alpha_{\text{LB}}} \sup_{v \in X} \frac{\tilde{\delta}_{\text{KL}}^{(1)}(v)}{\|v\|_X},$$

as well as

$$(3.6) \quad \Delta_{\text{KL}}^b(\mu, \omega) := \frac{1}{\alpha_{\text{LB}}} \sup_{v \in X} \frac{\delta_{\text{KL}}^b(v)}{\|v\|_X}, \quad b \in \{f, \ell\}.$$

3.2. Primal and dual error. We start by estimating primal and dual errors involving both KL and RB truncation, i.e.,

$$(3.7) \quad e(\mu, \omega) := u(\mu, \omega) - u_{N,K}(\mu, \omega), \quad \tilde{e}^{(1)}(\mu, \omega) := p^{(1)}(\mu, \omega) - p_{N,K}^{(1)}(\mu, \omega),$$

where u and p denote the exact (truth) primal and dual solution of (2.1) and (2.9), respectively. For a better readability and for notational compactness, we omit the parameters μ and ω in the following whenever it does not affect the understanding.

Proposition 3.1. *Setting $\Delta(\mu, \omega) := \Delta_{\text{RB}}(\mu, \omega) + \Delta_{\text{KL}}(\mu, \omega) + \Delta_{\text{KL}}^f(\mu, \omega)$, we get $\|e(\mu, \omega)\|_X \leq \Delta(\mu, \omega)$ for all $(\mu, \omega) \in \mathcal{M}$.*

Proof. We have for any $v \in X$ that

$$\begin{aligned} a(e, v) &= a(u, v) - a(u_{N,K}, v) \\ &= (f(v) - f^K(v)) + (a^K(u_{N,K}, v) - a(u_{N,K}, v)) + (f^K(v) - a^K(u_{N,K}, v)). \end{aligned}$$

The last term coincides with $a^K(e_{\text{RB}}, v) = r_{\text{RB}}(v)$. Testing with $v = e$ yields

$$\begin{aligned} \|e\|_X &\leq \alpha_{\text{LB}}^{-1} \frac{a(e, e)}{\|e\|_X} \\ &\leq \frac{|f(e) - f^K(e)|}{\alpha_{\text{LB}} \|e\|_X} + \frac{|a^K(u_{N,K}, e) - a(u_{N,K}, e)|}{\alpha_{\text{LB}} \|e\|_X} + \frac{|f^K(e) - a^K(u_{N,K}, e)|}{\alpha_{\text{LB}} \|e\|_X} \\ &\leq \Delta_{\text{KL}}^f + \Delta_{\text{KL}} + \Delta_{\text{RB}} \end{aligned}$$

by standard RB estimates. \square

Corollary 3.2. *Setting $\tilde{\Delta}^{(1)}(\mu, \omega) = \tilde{\Delta}^{(1)} := \tilde{\Delta}_{RB}^{(1)} + \tilde{\Delta}_{KL}^{(1)} + \Delta_{KL}^\ell$ yields the estimate $\|\tilde{e}^{(1)}(\mu, \omega)\|_X \leq \tilde{\Delta}^{(1)}(\mu, \omega)$ for all $\mu, \omega \in \mathcal{M}_K$.*

Proof. In a similar way as above we get for any $v \in X$ that

$$\begin{aligned} a(v, \tilde{e}^{(1)}) &= a(v, p^{(1)}) - a(v, p_{N,K}^{(1)}) \\ &= (\ell^K(v) - \ell(v)) + (a^K(v, p_{N,K}^{(1)}) - a(v, p_{N,K}^{(1)})) - (\ell^K(v) + a^K(v, p_{N,K}^{(1)})) \end{aligned}$$

and using $v = \tilde{e}^{(1)}$ yields the desired estimate. \square

The next step is to investigate the effectivities of the above estimators. To this end, we define the Riesz representations of primal and dual residual by

$$(3.8) \quad (\mathcal{E}_{RB}(\mu, \omega), v)_X = r_{RB}(v; \mu, \omega), \quad (\tilde{\mathcal{E}}_{RB}^{(1)}(\mu, \omega), v)_X = \tilde{r}_{RB}^{(1)}(v; \mu, \omega), \quad v \in X,$$

for $\mu \in \mathcal{D}$ and $\omega \in \Omega$. Since \mathcal{E}_{RB} is the Riesz representation, we have that $\|\mathcal{E}_{RB}(\mu, \omega)\|_X = \|r_{RB}(\mu, \omega)\|_{X'}$ and thus by definition

$$(3.9a) \quad \|\mathcal{E}_{RB}(\mu, \omega)\|_X = \alpha_{LB}(\mu, \omega) \Delta_{RB}(\mu, \omega),$$

$$(3.9b) \quad \|\tilde{\mathcal{E}}_{RB}^{(1)}(\mu, \omega)\|_X = \alpha_{LB}(\mu, \omega) \tilde{\Delta}_{RB}^{(1)}(\mu, \omega).$$

Analogously, we define the Riesz representations of the KL residuals by

$$(3.10a) \quad (\mathcal{E}_{KL}(\mu, \omega), v)_X = r(v; \mu, \omega) - r_{RB}(v; \mu, \omega),$$

$$(3.10b) \quad (\tilde{\mathcal{E}}_{KL}^{(1)}(\mu, \omega), v)_X = \tilde{r}(v; \mu, \omega) - \tilde{r}_{RB}^{(1)}(v; \mu, \omega),$$

where the truth residuals are defined as

$$(3.11a) \quad r(v; \mu, \omega) := f(v; \mu, \omega) - a(u_{N,K}, v; \mu, \omega),$$

$$(3.11b) \quad \tilde{r}(v; \mu, \omega) := -\ell(v; \mu, \omega) - a(v, p_{N,K}^{(1)}; \mu, \omega).$$

We obtain that

$$\begin{aligned} \|\mathcal{E}_{KL}\|_X &= \|r - r_{RB}\|_{X'} = \|f - a(u_{N,K}, \cdot) - f^K + a^K(u_{N,K}, \cdot)\|_{X'} \\ &\leq \|f - f^K\|_{X'} + \|a(u_{N,K}, \cdot) - a^K(u_{N,K}, \cdot)\|_{X'} = \alpha_{LB}(\mu, \omega) (\Delta_{KL}^f + \Delta_{KL}) \end{aligned}$$

and similarly $\|\tilde{\mathcal{E}}_{KL}^{(1)}\|_X \leq \alpha_{LB}(\Delta_{KL}^\ell + \tilde{\Delta}_{KL}^{(1)})$. Finally, in order to estimate the effectivities

$$(3.12) \quad \eta(\mu, \omega) := \frac{\Delta(\mu, \omega)}{\|e(\mu, \omega)\|_X}, \quad \tilde{\eta}^{(1)}(\mu, \omega) := \frac{\tilde{\Delta}^{(1)}(\mu, \omega)}{\|\tilde{e}^{(1)}(\mu, \omega)\|_X},$$

we define the following quantities

$$(3.13a) \quad c(\mu, \omega) := \frac{\Delta_{KL}(\mu, \omega) + \Delta_{KL}^f(\mu, \omega)}{\Delta_{RB}(\mu, \omega)},$$

$$(3.13b) \quad \tilde{c}^{(1)}(\mu, \omega) := \frac{\tilde{\Delta}_{KL}^{(1)}(\mu, \omega) + \Delta_{KL}^\ell(\mu, \omega)}{\tilde{\Delta}_{RB}^{(1)}(\mu, \omega)}.$$

Proposition 3.3. *If $c(\mu, \omega) \in [0, 1)$, we get*

$$\eta(\mu, \omega) \leq \frac{\gamma_{UB}(\mu, \omega)}{\alpha_{LB}(\mu, \omega)} \frac{1 + c(\mu, \omega)}{1 - c(\mu, \omega)},$$

where $\gamma_{UB}(\mu, \omega) \geq \gamma(\mu, \omega)$ is an upper continuity bound.

Proof. It is straightforward to see that for $v \in X$ we have

$$\begin{aligned} a(e, v) &= r(v; \mu, \omega) = r(v; \mu, \omega) - r_{\text{RB}}(v; \mu, \omega) + r_{\text{RB}}(v; \mu, \omega) \\ &= (\mathcal{E}_{\text{KL}}(\mu, \omega), v)_X + (\mathcal{E}_{\text{RB}}(\mu, \omega), v)_X = (\mathcal{E}_{\text{KL}}(\mu, \omega) + \mathcal{E}_{\text{RB}}(\mu, \omega), v)_X, \end{aligned}$$

thus, with $v = \mathcal{E}_{\text{RB}} - \mathcal{E}_{\text{KL}}$

$$a(e, \mathcal{E}_{\text{RB}} - \mathcal{E}_{\text{KL}}) = (\mathcal{E}_{\text{KL}} + \mathcal{E}_{\text{RB}}, \mathcal{E}_{\text{RB}} - \mathcal{E}_{\text{KL}})_X = \|\mathcal{E}_{\text{RB}}\|_X^2 - \|\mathcal{E}_{\text{KL}}\|_X^2,$$

hence

$$\begin{aligned} \|\mathcal{E}_{\text{RB}}\|_X^2 - \|\mathcal{E}_{\text{KL}}\|_X^2 &= a(e, \mathcal{E}_{\text{RB}} - \mathcal{E}_{\text{KL}}) \leq \gamma_{\text{UB}} \|e\|_X (\|\mathcal{E}_{\text{RB}}\|_X + \|\mathcal{E}_{\text{KL}}\|_X) \\ &= \gamma_{\text{UB}} \|e\|_X \frac{\|\mathcal{E}_{\text{RB}}\|_X^2 - \|\mathcal{E}_{\text{KL}}\|_X^2}{\|\mathcal{E}_{\text{RB}}\|_X - \|\mathcal{E}_{\text{KL}}\|_X}, \end{aligned}$$

i.e., by the above estimates

$$\|e\|_X \geq \frac{1}{\gamma_{\text{UB}}} (\|\mathcal{E}_{\text{RB}}\|_X - \|\mathcal{E}_{\text{KL}}\|_X) \geq \frac{\alpha_{\text{LB}}}{\gamma_{\text{UB}}} (\Delta_{\text{RB}} - \Delta_{\text{KL}} - \Delta_{\text{KL}}^f).$$

This finally implies that

$$\eta = \frac{\Delta}{\|e\|_X} \leq \frac{\gamma_{\text{UB}}}{\alpha_{\text{LB}}} \frac{\Delta_{\text{RB}} + \Delta_{\text{KL}} + \Delta_{\text{KL}}^f}{\Delta_{\text{RB}} - \Delta_{\text{KL}} - \Delta_{\text{KL}}^f} = \frac{\gamma_{\text{UB}}}{\alpha_{\text{LB}}} \frac{1+c}{1-c},$$

which proves the claim. \square

Completely analogously we can estimate the dual effectivity as follows.

Corollary 3.4. *If $\tilde{c}^{(1)}(\mu, \omega) \in [0, 1)$, we get*

$$\tilde{\eta}^{(1)}(\mu, \omega) \leq \frac{\gamma_{\text{UB}}(\mu, \omega)}{\alpha_{\text{LB}}(\mu, \omega)} \frac{1 + \tilde{c}^{(1)}(\mu, \omega)}{1 - \tilde{c}^{(1)}(\mu, \omega)}.$$

\square

Finally, for later reference, we note another result. Defining

$$(3.14) \quad \eta_0(\mu, \omega) := \sqrt{\frac{\gamma_{\text{UB}}(\mu, \omega)}{\alpha_{\text{LB}}(\mu, \omega)}} \left(\frac{1 + c(\mu, \omega)}{1 - c(\mu, \omega)} \right),$$

we get the following estimate for the effectivity w.r.t. the energy norm.

Corollary 3.5. *If $c(\mu, \omega) \in [0, 1)$, we get*

$$\frac{\sqrt{\alpha_{\text{LB}}(\mu, \omega)} \Delta(\mu, \omega)}{\|e(\mu, \omega)\|_{\mu, \omega}} \leq \eta_0(\mu, \omega).$$

Proof. In the proof of Proposition 3.3, we replace $\|e\|_X$ by $\|e\|_{\mu, \omega} \gamma_{\text{UB}}^{-1/2}$. \square

3.3. Output error. Now we consider the approximation $\ell^K(u_{N,K}; \mu, \omega)$ to the output $\ell(u; \mu, \omega) = s(\mu, \omega)$. As already known from the RB a-posteriori error analysis of linear output functionals, [15], we add a correction term and consider

$$(3.15) \quad s_{N,K}(\mu, \omega) := \ell^K(u_{N,K}; \mu, \omega) - r_{\text{RB}}(p_{N,K}^{(1)}; \mu, \omega)$$

and define the output error estimator by

$$(3.16) \quad \Delta^s := \alpha_{\text{LB}} \tilde{\Delta}^{(1)} + \delta_{\text{KL}}(p_{N,K}^{(1)}) + \delta_{\text{KL}}^f(p_{N,K}^{(1)}) + \delta_{\text{KL}}^\ell(u_{N,K}).$$

Then, we obtain the following estimate.

Theorem 3.6. *It holds $|s(\mu, \omega) - s_{N,K}(\mu, \omega)| \leq \Delta^s(\mu, \omega)$ for all $\mu \in \mathcal{D}$ and $\omega \in \Omega$.*

Proof. By standard arguments, we get (omitting the argument (μ, ω))

$$\begin{aligned} s - s_{N,K} &= \ell(u) - \ell^K(u_{N,K}) + r_{\text{RB}}(p_{N,K}^{(1)}) \\ &= \ell(u) - \ell^K(u_{N,K}) + f^K(p_{N,K}^{(1)}) - a^K(u_{N,K}, p_{N,K}^{(1)}) \\ &= [\ell^K(u) - \ell^K(u_{N,K})] + [f(p_{N,K}^{(1)}) - a^K(u_{N,K}, p_{N,K}^{(1)})] \\ &\quad + [\ell(u) - \ell^K(u)] - [f(p_{N,K}^{(1)}) - f^K(p_{N,K}^{(1)})]. \end{aligned}$$

For the first term on the right-hand side, we have

$$\ell^K(u) - \ell^K(u_{N,K}) = -a^K(u, p_K^{(1)}) + a^K(u_{N,K}, p_K^{(1)}) = -a^K(e, p_K^{(1)}).$$

Using $f(p_{N,K}^{(1)}) = a(u, p_{N,K}^{(1)})$, we get for the first two terms

$$\begin{aligned} &[\ell^K(u) - \ell^K(u_{N,K})] + [f(p_{N,K}^{(1)}) - a^K(u_{N,K}, p_{N,K}^{(1)})] = \\ &= -a^K(e, p_K^{(1)}) + a(u, p_{N,K}^{(1)}) - a^K(u_{N,K}, p_{N,K}^{(1)}) \\ &= -a^K(e, p_K^{(1)}) + a^K(u - u_{N,K}, p_{N,K}^{(1)}) + [a(u, p_{N,K}^{(1)}) - a^K(u, p_{N,K}^{(1)})] \\ &= -a^K(e, p_K^{(1)} - p_{N,K}^{(1)}) + [a(u, p_{N,K}^{(1)}) - a^K(u, p_{N,K}^{(1)})] \\ &= -a^K(e, \tilde{e}_{\text{RB}}^{(1)}) + [a(u, p_{N,K}^{(1)}) - a^K(u, p_{N,K}^{(1)})]. \end{aligned}$$

Putting all this together yields

$$(3.17) \quad \begin{aligned} s - s_{N,K} &= -a^K(e, \tilde{e}_{\text{RB}}^{(1)}) + [a(u, p_{N,K}^{(1)}) - a^K(u, p_{N,K}^{(1)})] \\ &\quad + [\ell(u) - \ell^K(u)] - [f(p_{N,K}^{(1)}) - f^K(p_{N,K}^{(1)})]. \end{aligned}$$

Using the triangle inequality, we have to estimate these 4 terms separately, i.e.,

$$|a^K(e, \tilde{e}_{\text{RB}}^{(1)})| = |\tilde{r}_{\text{RB}}^{(1)}(e; \mu, \omega)| \leq \|e\|_X \|\tilde{r}_{\text{RB}}^{(1)}\|_{X'} = \|e\|_X \alpha_{\text{LB}} \tilde{\Delta}_{\text{RB}}^{(1)} \leq \alpha_{\text{LB}} \Delta \tilde{\Delta}_{\text{RB}}^{(1)}$$

by Proposition 3.1. For the second term, we have

$$\begin{aligned} |a(u, p_{N,K}^{(1)}) - a^K(u, p_{N,K}^{(1)})| &\leq |a(e, p_{N,K}^{(1)}) - a^K(e, p_{N,K}^{(1)})| \\ &\quad + |a(u_{N,K}, p_{N,K}^{(1)}) - a^K(u_{N,K}, p_{N,K}^{(1)})| \\ &\leq \|e\|_X \|\tilde{\delta}_{\text{KL}}^{(1)}\|_{X'} + \delta_{\text{KL}}(p_{N,K}^{(1)}) \\ &\leq \alpha_{\text{LB}} \Delta \tilde{\Delta}_{\text{KL}}^{(1)} + \delta_{\text{KL}}(p_{N,K}^{(1)}) \end{aligned}$$

again by Proposition 3.1. Next,

$$|\ell(u) - \ell^K(u)| \leq |\ell(u_{N,K}) - \ell^K(u_{N,K})| + |\ell(e) - \ell^K(e)| \leq \delta_{\text{KL}}^\ell(u_{N,K}) + \alpha_{\text{LB}} \Delta \Delta_{\text{KL}}^\ell$$

and $|f(p_{N,K}^{(1)}) - f^K(p_{N,K}^{(1)})| \leq \delta_{\text{KL}}^f(p_{N,K}^{(1)})$. Putting everything together yields the desired result. \square

The above analysis shows two effects. First of all the RB and KL error terms in $\Delta = \Delta_{\text{RB}} + \Delta_{\text{KL}} + \Delta_{\text{KL}}^f$ and $\tilde{\Delta}^{(1)} = \tilde{\Delta}_{\text{RB}}^{(1)} + \tilde{\Delta}_{\text{KL}}^{(1)} + \Delta_{\text{KL}}^\ell$ are multiplied. In order to obtain the full order of approximation, RB and KL error terms should thus be of comparable sizes. Secondly, as opposed to the deterministic case, we obtain the additional additive terms $\delta_{\text{KL}}(p_{N,K}^{(1)})$, $\delta_{\text{KL}}^f(p_{N,K}^{(1)})$ and $\delta_{\text{KL}}^\ell(u_{N,K})$ as we see from the estimates of $|a(u, p_{N,K}^{(1)}) - a^K(u, p_{N,K}^{(1)})|$, $|f(p_{N,K}^{(1)}) - f^K(p_{N,K}^{(1)})|$ and $|\ell(u) - \ell^K(u)|$.

Finally, we investigate the effectivity of the output error bound for the special case of a compliant output, i.e., $\ell = f$, and symmetric bilinear form a . For this

case, we have $p_{N,K}^{(1)} = -u_{N,K}$, $\tilde{N}^{(1)} = N$ and $\Delta^s = \alpha_{LB} \Delta^2 + \delta_{KL}^{comp}$, $\delta_{KL}^{comp} := \delta_{KL}(u_{N,K}) + 2\delta_{KL}^f(u_{N,K})$.

Proposition 3.7. *In the compliant case and with symmetric bilinear form a and for $\eta_0(\mu, \omega)$ from (3.14), we assume that $\alpha_{LB}(\mu, \omega)\Delta(\mu, \omega)^2 \geq \eta_0(\mu, \omega)^2\delta_{KL}^{comp}(\mu, \omega)$. Then, the effectivity $\eta^s(\mu, \omega) := \frac{\Delta^s(\mu, \omega)}{|s(\mu, \omega) - s_{N,K}(\mu, \omega)|}$ is bounded by*

$$(3.18) \quad \eta^s(\mu, \omega) \leq \eta_0(\mu, \omega)^2 \frac{\alpha_{LB}(\mu, \omega)\Delta(\mu, \omega)^2 + \delta_{KL}^{comp}(\mu, \omega)}{\alpha_{LB}(\mu, \omega)\Delta(\mu, \omega)^2 - \eta_0(\mu, \omega)^2\delta_{KL}^{comp}(\mu, \omega)}.$$

Proof. Following the proof of Theorem 3.6 yields for $\ell = f$ and $p_{N,K}^{(1)} = -u_{N,K}$ that

$$\begin{aligned} s - s_{N,K} &= f(u) - 2f^K(u_{N,K}) + a^K(u_{N,K}, u_{N,K}) \\ &= a(u, u) + 2[f(u_{N,K}) - f^K(u_{N,K})] - 2f(u_{N,K}) + a(u_{N,K}, u_{N,K}) \\ &\quad - [a(u_{N,K}, u_{N,K}) - a^K(u_{N,K}, u_{N,K})] \\ &= a(e, e) + 2[f(u_{N,K}) - f^K(u_{N,K})] - [a(u_{N,K}, u_{N,K}) - a^K(u_{N,K}, u_{N,K})], \end{aligned}$$

Using Corollary 3.5, we get

$$\frac{\alpha_{LB}}{\eta_0^2} \Delta^2 \leq \|e\|_{\mu, \omega}^2 = a(e, e) \leq |s - s_{N,K}| + \delta_{KL}^{comp}.$$

This yields $\frac{\Delta^s}{|s - s_{N,K}|} \leq \frac{\alpha_{LB} \Delta^2 + \delta_{KL}^{comp}}{\frac{\alpha_{LB}}{\eta_0^2} \Delta^2 - \delta_{KL}^{comp}}$ which proves the claim. \square

The assumption $\alpha_{LB}(\mu, \omega)\Delta(\mu, \omega)^2 \geq \eta_0(\mu, \omega)^2\delta_{KL}^{comp}(\mu, \omega)$ is rather restrictive and can be validated only a-posteriori. It requires either the energy norm error effectivity η_0 or the KL truncation error δ_{KL}^{comp} to be small. However, the effectivity bound is consistent with the deterministic case in the sense that for large K , it converges to the energy norm error effectivity bound η_0^2 as provided in Corollary 3.5, where c is approaching zero at the same time.

3.4. Quadratic output. As a next step, we consider quadratic output functions of the form

$$s^2(\mu, \omega) := [\ell(u(\mu, \omega); \mu)]^2,$$

where ℓ is a ω -independent linear functional. If ℓ would be stochastic itself, the subsequently constructed error bounds would include terms depending on the size of s which is independent of N and K . Also, it is readily seen that just squaring the output $s_{N,K}$ from (3.15) is not sufficient. In fact, since

$$(3.19) \quad s^2 - (s_{N,K})^2 = (s - s_{N,K})(s + s_{N,K}) \leq \Delta^s \cdot (s + s_{N,K}),$$

the right-hand does not have the desirable ‘‘square’’ effect, as typical in RB methods. Hence, we follow a different path by introducing an additional dual problem, namely determine $p_K^{(2)}(\mu, \omega) \in X$ such that

$$(3.20) \quad a^K(v, p_K^{(2)}(\mu, \omega); \mu, \omega) = -2s_{N,K}(\mu, \omega) \cdot \ell(v; \mu) =: -\ell^{(2)}(v; \mu, \omega), \quad v \in X.$$

Of course, the solution of (3.20) reads $p_K^{(2)} = 2s_{N,K}p_K^{(1)}$, which, however, is useless in the RB context since we have a different parameter-dependent right-hand side and thus different RB spaces. Hence, we consider an RB space $\tilde{X}_N^{(2)} \subset X$, $\dim(\tilde{X}_N^{(2)}) = \tilde{N}^{(2)}$ and determine some $p_{N,K}^{(2)}(\mu, \omega) \in \tilde{X}_N^{(2)}$ such that

$$(3.21) \quad a^K(v, p_{N,K}^{(2)}(\mu, \omega); \mu, \omega) = -\ell^{(2)}(v; \mu, \omega), \quad v \in \tilde{X}_N^{(2)}.$$

We can apply the analysis performed in Section 3.2 and just need to adjust the notation. The dual error reads $\tilde{e}_{\text{RB}}^{(2)} := p_K^{(2)} - p_{N,K}^{(2)}$, the residual $\tilde{r}_{\text{RB}}^{(2)}(v) := a^K(v, \tilde{e}_{\text{RB}}^{(2)})$ and the RB bounds as $\tilde{\Delta}_{\text{RB}}^{(2)} := \alpha_{\text{LB}}^{-1} \sup_{v \in X} (\tilde{r}_{\text{RB}}^{(2)}(v) / \|v\|_X)$. The KL truncation term $\tilde{\delta}_{\text{KL}}^{(2)}$ is defined analogously to (3.4b) by replacing $p_{N,K}^{(1)}$ by $p_{N,K}^{(2)}$, and analogously to (3.5), $\tilde{\Delta}_{\text{KL}}^{(2)} := \alpha_{\text{LB}}^{-1} \sup_{v \in X} (\tilde{\delta}_{\text{KL}}^{(2)}(v) / \|v\|_X)$. The terms $\delta_{\text{KL}}^{\ell^{(2)}}(v; \mu)$ and $\Delta_{\text{KL}}^{\ell^{(2)}}(\mu, \omega)$ vanish since ℓ is deterministic. Then, Proposition 3.1 and Corollary 3.2 yield the following estimate for $\tilde{e}^{(2)} := p^{(2)} - p_{N,K}^{(2)}$, namely

$$(3.22) \quad \|\tilde{e}^{(2)}(\mu, \omega)\|_X \leq \tilde{\Delta}^{(2)}(\mu, \omega) := \tilde{\Delta}_{\text{RB}}^{(2)}(\mu, \omega) + \tilde{\Delta}_{\text{KL}}^{(2)}(\mu, \omega).$$

We consider the approximation $[\ell(u_{N,K}(\mu, \omega); \mu, \omega)]^2$. Similar to the definition of $s_{N,K}$ in Section 3.3, we add correction terms and consider

$$(3.23) \quad s_{N,K}^{[2]}(\mu, \omega) := (\ell(u_{N,K}))^2 - \left(r_{\text{RB}}(p_{N,K}^{(1)})\right)^2 - r_{\text{RB}}(p_{N,K}^{(2)}).$$

It is important to keep in mind that we distinguish the squared approximation $(s_{N,K})^2 = s_{N,K} \cdot s_{N,K}$ from the approximation $s_{N,K}^{[2]}$ of the square of s . In fact, it is easy to see that we can also write $s_{N,K}^{[2]}$ in terms of $s_{N,K} = \ell(u_{N,K}) - r_{\text{RB}}(p_{N,K}^{(1)})$,

$$(3.24) \quad s_{N,K}^{[2]}(\mu, \omega) = (s_{N,K})^2 + 2s_{N,K} \cdot r_{\text{RB}}(p_{N,K}^{(1)}) - r_{\text{RB}}(p_{N,K}^{(2)}),$$

i.e., we have two additional correction terms. For $\tilde{X}_N^{(2)} = \tilde{X}_N^{(1)}$, the correction terms would cancel out. We define the quadratic output error bound

$$(3.25) \quad \Delta^{s^2}(\mu, \omega) := (\Delta^s)^2 + \alpha_{\text{LB}} \Delta \tilde{\Delta}^{(2)} + \delta_{\text{KL}}(p_{N,K}^{(2)}) + \delta_{\text{KL}}^f(p_{N,K}^{(2)})$$

and obtain the following result.

Theorem 3.8. *It holds $|s^2(\mu, \omega) - s_{N,K}^{[2]}(\mu, \omega)| \leq \Delta^{s^2}(\mu, \omega)$ for all $\mu \in \mathcal{D}$, $\omega \in \Omega$.*

Proof. With (3.24), the output error is given by

$$\begin{aligned} s^2 - s_{N,K}^{[2]} &= s^2 - (s_{N,K})^2 - 2s_{N,K} r_{\text{RB}}(p_{N,K}^{(1)}) + r_{\text{RB}}(p_{N,K}^{(2)}) \\ &= (s - s_{N,K})^2 + 2s_{N,K}(s - s_{N,K}) - 2s_{N,K} r_{\text{RB}}(p_{N,K}^{(1)}) + r_{\text{RB}}(p_{N,K}^{(2)}). \end{aligned}$$

Using $s_{N,K} = \ell(u_{N,K}) - r_{\text{RB}}(p_{N,K}^{(1)})$ yields

$$2s_{N,K}(s - s_{N,K}) = 2s_{N,K} \left(\ell(u) - \ell(u_{N,K}) + r_{\text{RB}}(p_{N,K}^{(1)}) \right).$$

Together, replacing $2s_{N,K}\ell$ by $\ell^{(2)}$, we have

$$(3.26) \quad s^2 - s_{N,K}^{[2]} = (s - s_{N,K})^2 + \ell^{(2)}(u) - \ell^{(2)}(u_{N,K}) + r_{\text{RB}}(p_{N,K}^{(2)}).$$

From Theorem 3.6, we know that $(s - s_{N,K})^2 \leq (\Delta^s)^2$. The second part of (3.26) can be estimated analogously to Theorem 3.6 by replacing ℓ by $\ell^{(2)}$ and $p^{(1)}$ by $p^{(2)}$. Since $\ell = \ell^K$, we obtain

$$\left| \ell^{(2)}(u) - \ell^{(2)}(u_{N,K}) + r_{\text{RB}}(p_{N,K}^{(2)}) \right| \leq \alpha_{\text{LB}} \Delta \tilde{\Delta}^{(2)} + \delta_{\text{KL}}(p_{N,K}^{(2)}) + \delta_{\text{KL}}^f(p_{N,K}^{(2)}),$$

which proves the claim. \square

If Δ^s is already small, the first part of the error bound Δ^{s^2} will be comparatively negligible. The second part of the error bound is of the same form as Δ^s in (3.16). Hence, we can hope that Δ^{s^2} is approximately of the same order than Δ^s .

4. STATISTICAL OUTPUT ERROR ANALYSIS

In this section, we consider first and second moments of the linear output functional $s(\mu, \omega) = \ell(u(\mu, \omega); \mu)$,

$$\mathbb{M}_1(\mu) := \mathbb{E}[s(\mu, \cdot)], \quad \mathbb{M}_2(\mu) := \mathbb{E}[s^2(\mu, \cdot)], \quad \mathbb{V}(\mu) := \mathbb{M}_2(\mu) - (\mathbb{M}_1(\mu))^2.$$

We assume again that the functional ℓ is deterministic, i.e., there is no explicit dependence on the stochastic parameter ω but the randomness of the output functional s is only through u .

4.1. First and second moment. The straightforward estimate for the first moment $\mathbb{M}_1(\mu)$ is given by $\mathbb{M}_{1,NK}(\mu) := \mathbb{E}[s_{N,K}(\mu, \cdot)]$ and Theorem 3.6 yields the error bound

$$(4.27) \quad |\mathbb{M}_1(\mu) - \mathbb{M}_{1,NK}(\mu)| \leq \Delta^{\mathbb{M}_1}(\mu) := \mathbb{E}[\Delta^s(\mu, \cdot)].$$

Analogously, the straightforward estimate for the second moment $\mathbb{M}_2(\mu)$ is given by $\mathbb{M}_{2,NK}(\mu) := \mathbb{E}[s_{N,K}^{[2]}(\mu, \cdot)]$ and Theorem 3.8 yields the error bound

$$(4.28) \quad |\mathbb{M}_2(\mu) - \mathbb{M}_{2,NK}(\mu)| \leq \Delta^{\mathbb{M}_2}(\mu) := \mathbb{E}[\Delta^{s^2}(\mu, \cdot)].$$

4.2. Squared first moment. In order to get an estimation of the variance, it remains to find an estimation for the squared first moment. We follow the same approach as in Section 3.4 and introduce a third dual problem with right-hand side $\ell^{(3)}(v; \mu) := 2\mathbb{M}_{1,NK}(\mu)\ell(v; \mu)$. The dual and the corresponding reduced system are then given by

$$(4.29) \quad a^K(v, p_K^{(3)}; \mu, \omega) = -\ell^{(3)}(v; \mu), \quad v \in X,$$

$$(4.30) \quad a^K(v, p_{N,K}^{(3)}; \mu, \omega) = -\ell^{(3)}(v; \mu), \quad v \in \tilde{X}_N^{(3)},$$

respectively, where $\tilde{X}_N^{(3)} \subset X$ denotes the RB space of dimension $\dim(\tilde{X}_N^{(3)}) = \tilde{N}^{(3)}$. The error analysis is now mainly straightforward, following Section 3.4. We denote the new dual error by $\tilde{e}_{\text{RB}}^{(3)} := p_K^{(3)} - p_{N,K}^{(3)}$ and the residual by $\tilde{r}_{\text{RB}}^{(3)}(v) := a^K(v, \tilde{e}_{\text{RB}}^{(3)})$ to define the RB bound $\tilde{\Delta}_{\text{RB}}^{(3)} := \alpha_{\text{LB}}^{-1} \|\tilde{r}_{\text{RB}}^{(3)}\|_{X'}$. The KL truncation term $\tilde{\delta}_{\text{KL}}^{(3)}$ is defined analogously to (3.4b) by replacing $p_{N,K}^{(1)}$ by $p_{N,K}^{(3)}$, and analogously to (3.5), $\tilde{\Delta}_{\text{KL}}^{(3)} := \alpha_{\text{LB}}^{-1} \|\tilde{\delta}_{\text{KL}}^{(3)}\|_{X'}$. Then, Proposition 3.1 and Corollary 3.2 yield the following estimate for $\tilde{e}^{(3)} := p^{(3)} - p_{N,K}^{(3)}$,

$$(4.31) \quad \|\tilde{e}^{(3)}(\mu, \omega)\|_X \leq \tilde{\Delta}^{(3)}(\mu, \omega) := \tilde{\Delta}_{\text{RB}}^{(3)}(\mu, \omega) + \tilde{\Delta}_{\text{KL}}^{(3)}(\mu, \omega).$$

We define the approximation of the squared first moment adding some correction terms. Analogously to (3.24), we consider

$$(4.32) \quad \mathbb{M}_{1,NK}^{[2]}(\mu, \omega) = (\mathbb{M}_{1,NK})^2 + 2\mathbb{M}_{1,NK} \cdot \mathbb{E} \left[r_{\text{RB}}(p_{N,K}^{(1)}) \right] - \mathbb{E} \left[r_{\text{RB}}(p_{N,K}^{(3)}) \right].$$

Note the distinction between the squared approximation $(\mathbb{M}_{1,NK})^2 = \mathbb{M}_{1,NK} \cdot \mathbb{M}_{1,NK}$ and the direct approximation $\mathbb{M}_{1,NK}^{[2]}$ of the squared first moment. The error bound is given by

$$(4.33) \quad \Delta^{\mathbb{M}_1^2}(\mu, \omega) := (\Delta^{\mathbb{M}_1})^2 + \mathbb{E} \left[\alpha_{\text{LB}} \Delta \tilde{\Delta}^{(3)} + \delta_{\text{KL}}(p_{N,K}^{(3)}) + \delta_{\text{KL}}^f(p_{N,K}^{(3)}) \right].$$

Theorem 4.1. *It holds $|\mathbb{M}_1^2(\mu) - \mathbb{M}_{1,NK}^{[2]}(\mu)| \leq \Delta^{\mathbb{M}_1^2}(\mu)$ for all $\mu \in \mathcal{D}$.*

Proof. Analogously to Theorem 3.8, the output error is given by

$$\mathbb{M}_1^2 - \mathbb{M}_{1,NK}^{[2]} = (\mathbb{M}_1 - \mathbb{M}_{1,NK})^2 + \mathbb{E} \left[\ell^{(3)}(u) - \ell^{(3)}(u_{N,K}) + r_{\text{RB}}(p_{N,K}^{(3)}) \right]$$

From (4.27), we know $(\mathbb{M}_1 - \mathbb{M}_{1,NK})^2 \leq (\Delta^{\mathbb{M}_1})^2 = (\mathbb{E}[\Delta^s])^2$. Analogously to Theorem 3.6, replacing ℓ by $\ell^{(3)}$ and $p^{(1)}$ by $p^{(3)}$, we obtain

$$\left| \ell^{(3)}(u) - \ell^{(3)}(u_{N,K}) + r_{\text{RB}}(p_{N,K}^{(3)}) \right| \leq \alpha_{\text{LB}} \Delta \tilde{\Delta}^{(3)} + \delta_{\text{KL}}(p_{N,K}^{(3)}) + \delta_{\text{KL}}^f(p_{N,K}^{(3)})$$

and the claim follows directly. \square

4.3. Variance. It is straightforward to define

$$(4.34) \quad \mathbb{V}_{NK}(\mu) := \mathbb{M}_{2,NK}(\mu) - \mathbb{M}_{1,NK}^{[2]}(\mu)$$

and it is furthermore clear that $|\mathbb{V} - \mathbb{V}_{NK}| \leq \mathbb{E}[\Delta^s] + \Delta^{\mathbb{M}_1}$ is an upper bound for the error. However, we can derive more precise error bounds. Denoting $\tilde{r}_{\text{RB}}^{(4)}(v) := a^K(v, \tilde{e}_{\text{RB}}^{(2)} - \tilde{e}_{\text{RB}}^{(3)})$ and $\tilde{\Delta}_{\text{RB}}^{(4)} := \alpha_{\text{LB}}^{-1} \sup_{v \in X} (\tilde{r}_{\text{RB}}^{(4)}(v) / \|v\|_X)$ as well as defining the KL truncation term $\tilde{\delta}_{\text{KL}}^{(4)}$ by (3.4b), replacing $p_{N,K}^{(1)}$ by $(p_{N,K}^{(2)} - p_{N,K}^{(3)})$, and analogously to (3.5), $\tilde{\Delta}_{\text{KL}}^{(4)} := \alpha_{\text{LB}}^{-1} \sup_{v \in X} (\tilde{\delta}_{\text{KL}}^{(4)}(v) / \|v\|_X)$, we obtain $\|\tilde{e}^{(2)} - \tilde{e}^{(3)}\|_X \leq \tilde{\Delta}^{(4)} := \tilde{\Delta}_{\text{RB}}^{(4)} + \tilde{\Delta}_{\text{KL}}^{(4)}$ and the variance error bound

$$(4.35) \quad \begin{aligned} \Delta^{\mathbb{V}}(\mu, \omega) &:= \mathbb{E}[(\Delta^s)^2] + (\Delta^{\mathbb{M}_1})^2 + \mathbb{E}[\alpha_{\text{LB}} \Delta \tilde{\Delta}^{(4)}] \\ &+ \mathbb{E}[\delta_{\text{KL}}(p_{N,K}^{(2)} - p_{N,K}^{(3)}) + \delta_{\text{KL}}^f(p_{N,K}^{(2)} - p_{N,K}^{(3)})] \end{aligned}$$

Proposition 4.2. *It holds that $|\mathbb{V}(\mu) - \mathbb{V}_{NK}(\mu)| \leq \Delta^{\mathbb{V}}(\mu)$ for all $\mu \in \mathcal{D}$.*

Proof. From Theorems 3.8 and 4.1 we know

$$\begin{aligned} \mathbb{V} - \mathbb{V}_{NK} &= \mathbb{E}[(s - s_{N,K})^2] - (\mathbb{M}_1 - \mathbb{M}_{1,NK})^2 \\ &+ \mathbb{E}[\ell^{(2)}(u) - \ell^{(2)}(u_{N,K}) + r_{\text{RB}}(p_{N,K}^{(2)})] \\ &- \mathbb{E}[\ell^{(3)}(u) - \ell^{(3)}(u_{N,K}) + r_{\text{RB}}(p_{N,K}^{(3)})] \end{aligned}$$

and the first two terms can be bounded by $\mathbb{E}[(\Delta^s)^2]$ and $(\Delta^{\mathbb{M}_1})^2$, respectively. Analogously to Theorem 3.6, we transform the other two expressions to the form of (3.17) and obtain

$$\begin{aligned} \ell^{(i)}(u) - \ell^{(i)}(u_{N,K}) + r_{\text{RB}}(p_{N,K}^{(i)}) &= -a^K(e, \tilde{e}_{\text{RB}}^{(i)}) + [a(u, p_{N,K}^{(i)}) - a^K(u, p_{N,K}^{(i)})] \\ &- [f(p_{N,K}^{(i)}) - f^K(p_{N,K}^{(i)})], \quad i = 2, 3. \end{aligned}$$

We subtract the two expressions and follow again the proof of Theorem 3.6. The claim follows directly using the definitions from above. \square

In our numerical experiments, we have observed that it is sufficient to use the same reduced space for the third dual problem (4.30) as for the second dual problem (3.21), i.e. $\tilde{X}_N^{(2)} = \tilde{X}_N^{(3)}$. Then, it is sufficient to solve only one additional dual problem and it holds that $p_{N,K}^{(3)}(\mu, \omega) = p_{N,K}^{(2)}(\mu, \omega) \mathbb{M}_{1,NK}(\mu) / s_{N,K}(\mu, \omega)$. Hence, we consider

$$(4.36) \quad a^K(v, p_{N,K}^{(4)}(\mu, \omega); \mu, \omega) = -2\ell(v; \mu), \quad v \in \tilde{X}_N^{(2)}$$

such that $p_{N,K}^{(2)} = s_{N,K} \cdot p_{N,K}^{(4)}$ and $p_{N,K}^{(3)} = \mathbb{M}_{1,NK} \cdot p_{N,K}^{(4)}$. For the evaluation of the variance error bound (4.35), we therefore use $p_{N,K}^{(2)} - p_{N,K}^{(3)} = (s_{N,K} - \mathbb{M}_{1,NK}) p_{N,K}^{(4)}$.

5. OFFLINE-ONLINE DECOMPOSITION

In this section, we describe the offline and online procedures and provide corresponding run-time and storage complexities. We start with the description of a method to evaluate lower bounds for the coercivity constant. For this method, we assume the bilinear form a to be parametrically coercive with respect to the deterministic parameter, i.e. $\theta_q^a(\mu) > 0$ for all $\mu \in \mathcal{D}$ and $\bar{a}_q(v, v) + a_q(v, v; \omega) \geq 0$, $v \in X$, for all $\omega \in \Omega$ and $1 \leq q \leq Q^a$.

5.1. The Coercivity Lower Bound. From the deterministic case, we know the following methods to determine lower bounds $\alpha_{LB}(\mu, \omega)$ for $\alpha(\mu, \omega)$, the “min- θ ” approach [15] and the “Successive Constraint Method” (SCM) [11]. The latter approach is less restrictive and could be directly applied to the stochastic parameter case. However, it requires much more effort, online as well as offline. The “min- θ ” approach requires the bilinear form a to be parametrically coercive with respect to the deterministic and stochastic parameter. Therefore, the extension of the method to our case is not possible. We would require $\xi_{q,k}(\omega)$ to be positive.

To partially maintain the advantage of the “min- θ ” approach, we propose a combination of both methods. We fix some parameter $\bar{\mu} \in \mathcal{D}$ and get the inequality

$$(5.1) \quad \alpha(\mu, \omega) = \inf_{v \in X} \frac{a(v, v; \mu, \omega)}{\|v\|_X^2} \geq \inf_{v \in X} \frac{a(v, v; \mu, \omega)}{a(v, v; \bar{\mu}, \omega)} \cdot \inf_{v \in X} \frac{a(v, v; \bar{\mu}, \omega)}{\|v\|_X^2}.$$

If a is parametrically coercive, we apply the “min- θ ” approach on the first term, i.e., for $\theta_{\min}(\mu) := \min_{1 \leq q \leq Q^a} \{\theta_q^a(\mu) / \theta_q^a(\bar{\mu})\}$, we obtain ω -independent lower bounds

$$\frac{a(v, v; \mu, \omega)}{a(v, v; \bar{\mu}, \omega)} \geq \theta_{\min}(\mu), \quad \forall v \in X, \forall (\mu, \omega) \in \mathcal{M}$$

analogously to [15]. For the approximation of second term, we first apply the SCM to the truncated form and obtain μ -independent lower bounds

$$\frac{a^K(v, v; \bar{\mu}, \omega)}{\|v\|_X^2} \geq \alpha_{SCM}^K(\omega), \quad \forall v \in X, \forall \omega \in \Omega.$$

To take the truncation error into account, we consider the parameter independent truncation error

$$(5.2) \quad \Delta_{KL}^\alpha := \sup_{v \in X} \left(\sum_{q=1}^{Q^a} \theta_q^a(\bar{\mu}) \sum_{k=K+1}^{K_{\max}} \xi_{UB} \frac{a_{q,k}(v, v)}{\|v\|_X^2} \right)$$

such that $-\Delta_{KL}^\alpha \|v\|_X^2 \leq a(v, v; \bar{\mu}, \omega) - a^K(v, v; \bar{\mu}, \omega)$. Hence, we define $\alpha_{SCM}(\omega) := \alpha_{SCM}^K(\omega) - \Delta_{KL}^\alpha$ and obtain the coercivity lower bound $\alpha_{LB}(\mu, \omega) := \theta_{\min}(\mu) \cdot \alpha_{SCM}(\omega)$. It is essential that K is large enough to obtain a positive α_{SCM} .

Both $\alpha_{SCM}(\omega)$ and $\theta_{\min}(\mu)$ can be evaluated independently. Therefore, in the offline stage, it might be useful to evaluate and store α_{SCM} for many ω and use these values in the online stage in combination with different μ . This is possible if the online required stochastic parameters can be fixed *a-priori*, for example using (Quasi) Monte Carlo methods. Then $\alpha_{LB}(\mu, \omega)$ can be evaluated very fast in the online stage.

5.2. Online Procedure. We first summarize the run-time complexity to solve a reduced system and evaluate the corresponding outputs and bounds. Assuming the availability of all necessary terms, the complexity is the same for all primal and dual problems. For notational compactness, we do not distinguish between Q^b , K^b , K_{\max}^b for $b \in \{a, f, \ell\}$, but just use Q , K and K_{\max} , respectively. In the same way, we just use N instead of N , $\tilde{N}^{(1)}$, $\tilde{N}^{(2)}$ and $\tilde{N}^{(3)}$.

The complexity to assemble a reduced systems for a new parameter pair reads $\mathcal{O}(QKN^2)$, the solution is then obtained in $\mathcal{O}(N^3)$ operations. For the output evaluation, we need to assemble some additional matrices and vectors — again with complexity $\mathcal{O}(QKN^2)$ — to evaluate the residuals. The actual evaluation is then of complexity $\mathcal{O}(N^2)$. For the error bounds, we first evaluate the coercivity lower bound. The complexity depends on the chosen method, optimally $\mathcal{O}(Q)$. For the Δ_{KL} - and Δ_{RB} -error bounds, we use the previously evaluated and stored Riesz representator inner products and compute the bounds in $\mathcal{O}(Q^2(K_{\max} - K)^2N^2)$ and $\mathcal{O}(Q^2K^2N^2)$, respectively. For the δ_{KL} -error bounds, we just need $\mathcal{O}(Q(K_{\max} - K))$ matrix-vector and vector-vector multiplications, the total complexity is therefore $\mathcal{O}(Q(K_{\max} - K)N^2)$.

Suppose we use M random realizations to evaluate the Monte Carlo estimates for any given deterministic parameter, the overall run-time complexity for the computation of $\mathbb{M}_{1,NK}$ and $\mathbb{M}_{2,NK}$ is given by $\mathcal{O}(M(N^3 + Q^2K_{\max}^2N^2))$, including the complexity for the evaluation of the error bounds.

If we are interested in both second moment and variance, the online procedure works as follows. We solve the primal and first dual problem for M realizations and some fixed μ . For all realizations, we store $s_{N,K}$ that is later used to solve the second and third dual problem (3.21) and (4.30). For the quadratic output evaluations, we additionally store $r_{\text{RB}}(p_{N,K}^{(1)})$ as well as the primal solutions $u_{N,K}$ that is needed for the computation of the respective last terms in (3.24) and (4.32). Furthermore, for the corresponding error bounds (3.25) and (4.35), we store Δ and Δ^s . Hence, the overall storage complexity is $\mathcal{O}((N + 4)M)$.

If M is large and storage is limited, it is possible to store only expectations and recompute the quantities $u_{N,K}$, $s_{N,K}$, $r_{\text{RB}}(p_{N,K}^{(1)})$, Δ and Δ^s when needed. The storage complexity can thus be reduced to $\mathcal{O}(1)$. However, the run-time will considerably increase.

Alternatively, using the the less precise variance error bound

$$|\mathbb{V} - \mathbb{V}_{NK}| \leq \Delta^{\mathbb{M}_2} + \Delta^{\mathbb{M}_1^2},$$

it is also possible to solve all problems without any recomputations and a storage complexity of only $\mathcal{O}(1)$, independent of N and M . The basic concept is to use just one additional dual space $\tilde{X}_N^{(2)}$ and solve the additional dual problem (4.36) at the same time as the primal and first dual problem (2.15) and (2.16). It is clear that the evaluation of $s_{N,K}^{[2]}$ in (3.24) and the second moment $\mathbb{M}_{2,NK} = \mathbb{E}[s_{N,K}^{[2]}]$ as well as its error bounds Δ^{s^2} from (3.25) and $\Delta^{\mathbb{M}_2} = \mathbb{E}[\Delta^{s^2}]$ can be obtained with storage complexity $\mathcal{O}(1)$. As a consequence of the use of (4.36), we have $\mathbb{E}[r_{\text{RB}}(p_{N,K}^{(3)})] = \mathbb{M}_{1,NK} \mathbb{E}[r_{\text{RB}}(p_{N,K}^{(4)})]$ and the evaluation of $\mathbb{M}_{1,NK}^{[2]}$ in (4.32) is of storage complexity $\mathcal{O}(1)$, too, and hence the evaluation of $\mathbb{V}_{NK} = \mathbb{M}_{2,NK} - \mathbb{M}_{1,NK}^{[2]}$. It remains to show that the storage complexity to evaluate $\Delta^{\mathbb{M}_1^2}$ in (4.33) is constant. We therefore have to separate $\mathbb{M}_{1,NK}$ -dependent and $p_{N,K}^{(4)}$ -dependent terms. It is

clear that $\delta_{\text{KL}}(p_{N,K}^{(3)}) = |\mathbb{M}_{1,NK}| \cdot \delta_{\text{KL}}(p_{N,K}^{(4)})$ and consequently $\mathbb{E}[\delta_{\text{KL}}(p_{N,K}^{(3)})] = |\mathbb{M}_{1,NK}| \cdot \mathbb{E}[\delta_{\text{KL}}(p_{N,K}^{(4)})]$. Since $\tilde{r}_{\text{RB}}^{(3)}(v) = \mathbb{M}_{1,NK} \cdot a^K(v, p^{(4)} - p_{N,K}^{(4)})$, we also have $\tilde{\Delta}_{\text{RB}}^{(3)} = |\mathbb{M}_{1,NK}| \cdot \alpha_{\text{LB}}^{-1} \sup_{v \in X} (a^K(v, p^{(4)} - p_{N,K}^{(4)}) / \|v\|_X)$ and analogously $\tilde{\Delta}_{\text{KL}}^{(3)} := |\mathbb{M}_{1,NK}| \cdot \alpha_{\text{LB}}^{-1} \sup_{v \in X} (\tilde{\delta}_{\text{KL}}^{(4)}(v) / \|v\|_X)$. Hence, $\mathbb{E}[\alpha_{\text{LB}} \Delta \tilde{\Delta}^{(3)}]$ can be separated and the storage complexity for the evaluation is $\mathcal{O}(1)$.

5.3. Greedy basis selection. To generate the bases of the reduced spaces, we perform a Greedy algorithm as it is well known in the RB context, [20, 15]. For a training parameter set $\Xi_{\text{train}} \subset \mathcal{M}$ and some initial basis, given by an arbitrary single snapshot, we solve the reduced primal and dual problems (2.15), (2.16), (3.21), (4.30) and evaluate the error bounds for the desired outputs. For each problem, we select the parameter pair for which the RB error part of the desired output error bound is maximal and add the corresponding solution of the unreduced problem to the respective basis. We iterate the procedure until the error bounds fall below an intended tolerance for all training parameters.

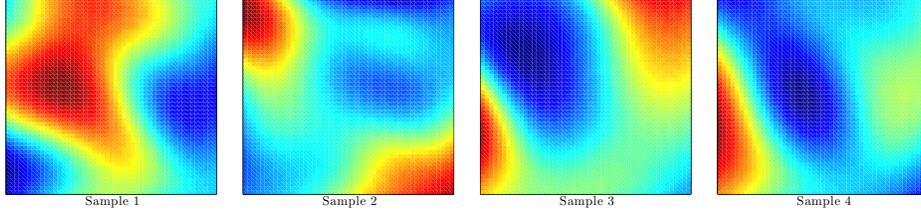
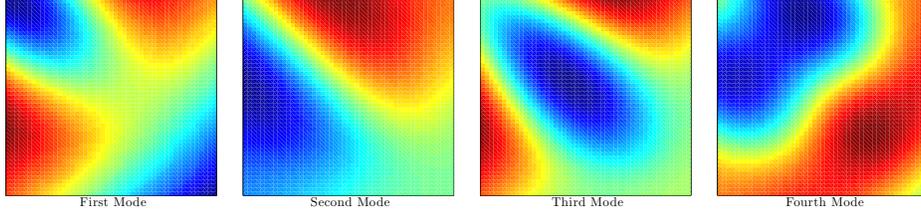
Next, we are going to describe how to specify the KL truncation, precisely the numbers of affine terms used for the approximation, K^b , $b \in \{a, f, \ell\}$, and the number of terms used to estimate the truncation error, K_{max}^b , $b \in \{a, f, \ell\}$. We integrate the specification into the Greedy algorithm. For different truncation lengths and very large K_{max} values, we solve the reduced system and evaluate the KL error bounds for all training parameters. K^b , $b \in \{a, f, \ell\}$, are chosen as the minimal numbers such that the KL error bounds do not exceed a given tolerance, respectively. This tolerance should be rather small compared to the allowed output errors. Similarly, we adjust K_{max}^b , $b \in \{a, f, \ell\}$, as small as possible such that we underestimate the KL error bounds only negligible small. Since the KL truncation errors do not depend on the dimension of the RB spaces, K^b and K_{max}^b , $b \in \{a, f, \ell\}$, are likely to be appropriate for all reduced spaces and can be fixed for all further computations. However, it would also be possible to do further adjustments during the Greedy algorithm.

Suppose that Ξ_{train} consists of n_{train} deterministic parameters and M_{train} random realizations for each of the parameters. Then, the Greedy complexity is $\mathcal{O}(Nn_{\text{train}})$ times the online complexity to find the ‘‘optimal’’ parameters in each iteration, i.e. $\mathcal{O}(Nn_{\text{train}}M_{\text{train}}(N^3 + Q^2K_{\text{max}}^2N^2))$, plus $\mathcal{O}(QK_{\text{max}}N\mathcal{N})$ to solve for the corresponding true solutions. Furthermore, the construction of the reduced system matrices and vectors is of complexity $\mathcal{O}(QK_{\text{max}}N^2\mathcal{N})$ and the evaluation of the used Riesz representators and the pairwise inner products $\mathcal{O}(Q^2K_{\text{max}}^2N^2\mathcal{N})$.

We store these RB system matrices and vectors as well as the Riesz representator inner products that are used to construct the Δ_{KL} - and Δ_{RB} -error bounds. Hence the total storage complexity is $\mathcal{O}(Q^2K_{\text{max}}^2N^2)$.

6. NUMERICAL REALIZATION AND EXPERIMENTS

In this section, an example of a two-dimensional porous medium is chosen to illustrate the different aspects of the proposed methods. We consider heat transfer in a wet sandstone with porosity modeled by a random function $\kappa(x; \omega)$ that represents the rate of pore space within some control volume and is assumed to be smooth in space. Furthermore, our model depends on a deterministic parameter $\mu \in \mathcal{D} = [0.01, 1]$ that denotes the global water saturation in the pores. Hence, the proportion of air in the pores is given by $(1 - \mu)$. Let $c_s = 2.40$ be the heat

FIGURE 6.1. Four random realizations of κ FIGURE 6.2. First four modes of $\tilde{\kappa}$

conductivity constant of pure (theoretically imporous) sandstone and $c_w = 0.60$, $c_a = 0.03$ the respective heat conductivity constants of water and air. With these notations, the total heat conductivity of a wet sandstone is assumed to be

$$(6.1) \quad \begin{aligned} c(x; \mu, \omega) &= c_s \cdot (1 - \kappa(x; \omega)) + (\mu c_w + (1 - \mu)c_a)\kappa(x; \omega) \\ &= c_s + (-c_s + \mu c_w + (1 - \mu)c_a)\kappa(x; \omega). \end{aligned}$$

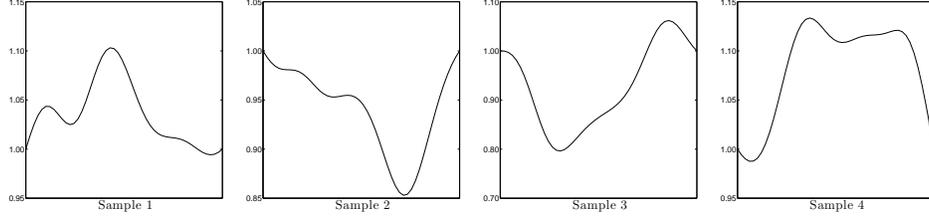
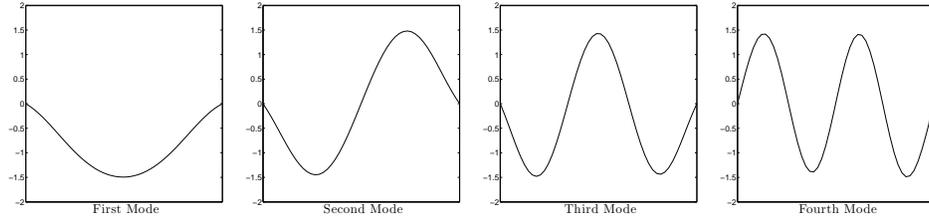
We consider a domain $D = [0, 1]^2$ and impose homogeneous Dirichlet boundary conditions on some boundary part Γ_D and non-homogeneous Neumann boundary conditions on the opposite “output” boundary Γ_{out} , where the right-hand side of the boundary condition is a random function $g(\omega) : [0, 1] \rightarrow \mathbb{R}$, representing some random loss of heat at the output boundary. On the other boundaries, we impose homogeneous Neumann conditions, representing isolated parts of the sandstone. For a given $\mu \in \mathcal{D}$ and some random realization of κ , we are interested in the average temperature at the “output” boundary Γ_{out} , denoted by $s(\mu, \omega)$.

Now, the PDE reads as follows: for given $(\mu, \omega) \in \mathcal{M}$, find $u(\mu, \omega)$ such that

$$(6.2) \quad \begin{cases} -\nabla \cdot (c(\mu, \omega) \nabla u(\mu, \omega)) &= 0 & \text{in } D, \\ u(\mu, \omega) &= 0 & \text{on } \Gamma_D, \\ n \cdot (c(\mu, \omega) \nabla u(\mu, \omega)) &= 0 & \text{on } \Gamma_N, \\ n \cdot (c(\mu, \omega) \nabla u(\mu, \omega)) &= g(\omega) & \text{on } \Gamma_{\text{out}}. \end{cases}$$

In the weak form, we compute $u(\mu, \omega) \in X$ such that $a(u(\mu, \omega), v; \mu, \omega) = f(v; \omega)$ for all $v \in X$, where $a(w, v; \mu, \omega) = \int_D c(\mu, \omega) \nabla w \cdot \nabla v$ and $f(v; \omega) = \int_{\Gamma_{\text{out}}} g(\omega) v$. For the functional $\ell(v) = \int_{\Gamma_{\text{out}}} v$, the non-compliant output is given by $s(\mu, \omega) := \ell(u(\mu, \omega))$.

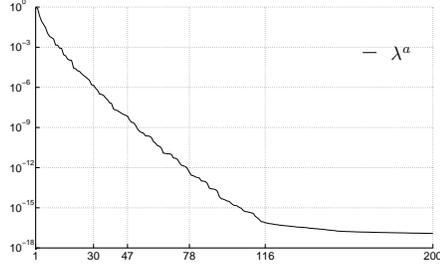
The affine decomposition of the bilinear form a in μ is straightforward. Let $\bar{\kappa}(x)$ denote the mean of $\kappa(x; \cdot)$ and $\tilde{\kappa}(x; \omega) := \kappa(x; \omega) - \bar{\kappa}(x)$ its stochastic part with zero mean. We define $\theta_1(\mu) := c_s$ and $\theta_2(\mu) := -c_s + \mu c_w + (1 - \mu)c_a$.


 FIGURE 6.3. Four random realizations of g

 FIGURE 6.4. First four modes of \tilde{g}

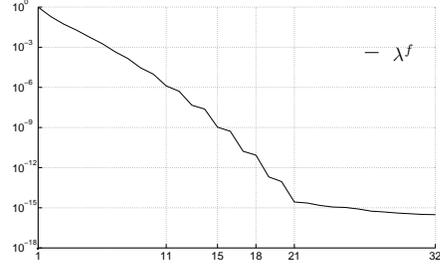
Then, using the notation of (2.2), $\bar{a}_1(w, v) = \int_D \nabla w \cdot \nabla v$ whereas $a_1(w, v; \omega) \equiv 0$ vanishes. For the second affine term, we have $\bar{a}_2(w, v) = \int_D \bar{\kappa} \nabla w \cdot \nabla v$ and $a_2(w, v; \omega) = \int_D \tilde{\kappa}(\omega) \nabla w \cdot \nabla v$. In the same way, we denote by $\bar{g}(x)$ the mean of $g(x; \cdot)$ and $\tilde{g}(x; \omega)$ its stochastic part and define $\bar{f}_1(v) = \int_{\Gamma_{\text{out}}} \bar{g} v$ as well as $f_1(v; \omega) = \int_{\Gamma_{\text{out}}} \tilde{g}(\omega) v$, where $\theta_1^f = 1$. Using KL expansions of $\tilde{\kappa}$ and \tilde{g} , we directly obtain affine decompositions of a_2 and f_1 in ω , respectively. Since ℓ is independent of μ and ω , we put all forms into the framework of (2.11) with $Q^a = 2$, $Q^f = 1$ and $Q^\ell = 1$, where $\xi_{1,k}^a(\omega) = 0$ for all $k \geq 1$ and therefore $K_1^a = 0$ in (2.12).

Figure 6.1 shows four random realizations of κ and Figure 6.2 the first four eigenmodes of the KL expansion of $\tilde{\kappa}$. Its eigenvalues are provided in Figure 6.5(a). The expectation of κ is supposed to be constant in space, $\bar{\kappa}(x) \equiv 0.33$. We assume the random coefficients $\xi_{2,k}^a(\omega)$ to be standard normally distributed. Since $\kappa(x; \omega)$ is restricted to $[0, 1]$ whereas $\xi_{2,k}^a(\omega)$ are unbounded, we dismiss realizations that do not satisfy the physical constraints. However, this can be done easily online and this happens with a probability of less than $2.5 \cdot 10^{-6}$ in our model. Then, $c(x; \mu, \omega) > \mu c_w + (1 - \mu) c_a > 0.0357 > 0$ and the PDE is uniformly coercive. Figure 6.3 shows four random realizations of g and Figure 6.4 the first four eigenmodes of the KL expansion of \tilde{g} . Its eigenvalues are provided in Figure 6.5(b). The expectation of g is constant in space, $\bar{g}(x) = 1$. The random coefficients $\xi_{1,k}^f(\omega)$ are assumed to be standard normally distributed. Here, we do not restrict g to a certain interval. However, negative values of g are very unlikely.

For the ‘‘truth’’ approximations, we choose a finite element (FE) space X with linear Lagrange elements and $\mathcal{N} = 4841$ degrees of freedom. Furthermore, we use $K_{\text{truth}}^a = 78$ and $K_{\text{truth}}^f = 18$ terms to assemble the ‘‘true’’ forms a and f , respectively. These numbers of terms are already precise enough compared to the FE error.

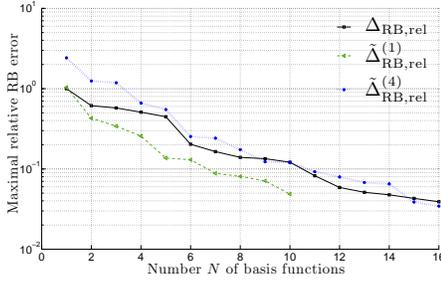


(a) Eigenvalues of the KL expansion of $\tilde{\kappa}$ and KL truncation values $K^a = 30$, $K_{\max}^a = 47$ and $K_{\text{truth}}^a = 78$

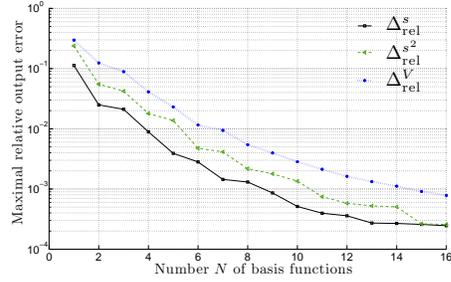


(b) Eigenvalues of the KL expansion of \tilde{g} and KL truncation values $K^f = 11$, $K_{\max}^f = 15$ and $K_{\text{truth}}^f = 18$

FIGURE 6.5. Eigenvalues and truncation values of the Karhunen-Loève expansions



(a) Relative error decay of primal solution u and dual solution $p^{(1)}$, and of $p^{(4)}$



(b) Relative error decay of outputs s , s^2 and V without δ_{KL} -contributions, respectively

FIGURE 6.6. Greedy error decay

The bilinear form a with the affine decomposition introduced before is not parametrically coercive since $\theta_2^a(\mu) < 0$. However, since $\bar{a}_2(\cdot) = 0.33 \cdot \bar{a}_1(\cdot)$, resorting the affine terms to

$$a(\cdot; \mu, \omega) = \theta_1^a(\mu)(\bar{a}_1(\cdot) - \bar{a}_2(\cdot) - a_2(\cdot; \omega)) + (\theta_1^a(\mu) + \theta_2^a(\mu))(\bar{a}_2(\cdot) + a_2(\cdot; \omega))$$

leads to a decomposition that fulfills the requirements of the proposed method to evaluate coercivity lower bounds.

Using the initial basis of the Greedy algorithm, we specify the KL truncation as described in Section 5.3. For a relative error tolerance $tol = 10^{-3}$, we choose a K^a and K^f such that the truncation errors, especially the δ_{KL} -parts, do not exceed $0.2tol$. This leads to $K^a = 30$, $K_{\max}^a = 47$, $K^f = 11$ and $K_{\max}^f = 15$, as marked in Figures 6.5(a) and 6.5(b). For the KL error bounds, we use the upper bound $\xi_{\text{UB}} := 5.2$ such that $|\xi_{q,k}| > \xi_{\text{UB}}$ with a probability of less than $2.5 \cdot 10^{-7}$.

As mentioned, we use the same space for the second and third dual space, $\tilde{X}_N^{(2)} = \tilde{X}_N^{(3)}$, and solve only the additional dual problem (4.36). Figure 6.6(a) shows the decay of the maximal relative error bounds of the primal and dual solutions u and $p^{(1)}$, and of the difference of the additional dual solutions $p^{(2)} - p^{(3)}$ that is used for

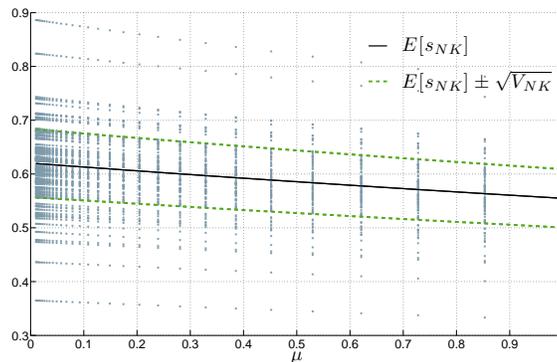


FIGURE 6.7. Mean output $\mathbb{E}[s_{N,K}(\mu, \cdot)]$, its standard deviation, and 100 random samples for a test set of 30 logarithmically distributed values of μ , respectively

the construction of the variance. In Figure 6.6(b) we provide the decay of the error bounds of the desired outputs. We omit the δ_{KL} -parts since they do not decrease with the number of basis functions and could therefore have a negative effect on the basis selection procedure. It turns out that $(N, \tilde{N}^{(1)}, \tilde{N}^{(2)}) = (16, 10, 16)$ is sufficient for relative error below the tolerance for all outputs.

On our reference system, a 3.06 GHz Intel Core 2 Duo processor, 4 GB RAM, we used Matlab 7.8.0 (R2009a) to implement and run both the truth and reduced model. Solving the truth with $\mathcal{N} = 4841$ degrees of freedom, we needed about 0.132 seconds per sample on average whereas the reduced problem could be solved in about 0.0105 second per sample, including the solution of all primal and dual problems and the evaluation of all outputs and error bounds. Hence, we gain a speedup by a factor greater than 12. To show that the number of reduced basis functions is independent of the degrees of freedom of the truth, we started another Greedy algorithm using $\mathcal{N} = 19121$. Again, the error bounds fell below the desired error tolerance for $(N, \tilde{N}^{(1)}, \tilde{N}^{(2)}) = (16, 10, 16)$. On average, the computation of the larger truth needed about 0.594 seconds per sample. Since the size of the reduced system did not change, we gain a speedup by a factor greater than 56.

The result of the reduced computation is shown in Figure 6.7. For each parameter of a test set of 30 logarithmically distributed values of μ , we evaluated the output s , its mean, and the variance \mathbb{V} using 10000 random samples. In Figure 6.7, we plotted the mean and standard deviation of $s_{N,K}$ as well as 100 random samples for each parameter of the test set.

In Figure 6.8, we show the errors and error bounds for the output s for two values of μ and 200 random samples each. The samples are sorted according to Δ^s . We see that the error bound is effective. The average effectivity $\Delta^s/|s - s_{N,K}|$ is about 100. We furthermore separated the error bound in its different parts. One can see that the δ_{KL} -part does hardly varies since it is not directly dependent on the current random realization. While for $\mu = 0.01$, $\alpha_{\text{LB}}\Delta\tilde{\Delta}^{(1)}$ contributes most to Δ^s , the δ_{KL} -parts contribute most for $\mu = 1.00$. Hence, adaptive choices of K^a and K^f could improve the error bounds and reduce the run-time and will be a part of future work.

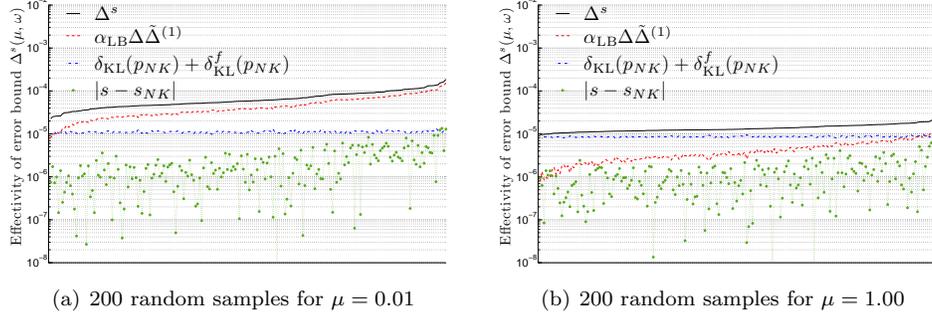


FIGURE 6.8. Error bound Δ^s , splitted in its δ_{KL} - and Δ -part, and true error of output s for 200 random samples and two values of μ

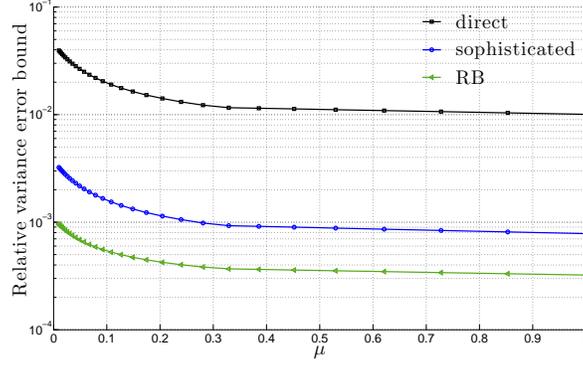


FIGURE 6.9. Different relative error bounds for variance $\mathbb{V}(\mu)$

In Figure 6.9 we compare our variance evaluation method and corresponding error bounds with two other evaluation procedures based upon the use of the sample variance $\mathbb{E}[(s_{N,K})^2] - (\mathbb{E}_{N,K})^2$. For the “direct” bound, we follow (3.19) and replace s by $(s - s_{N,K}) + s_{N,K}$ which can be estimated by $\Delta^s + |s_{N,K}|$. Analogously, we obtain $|\mathbb{M}_1| \leq \Delta^{\mathbb{M}_1} + |\mathbb{M}_{1,NK}|$ which leads us to the “direct” variance error bound

$$|\mathbb{V} - \mathbb{V}_{NK}| \leq \mathbb{E}[\Delta^s(\Delta^s + 2|s_{N,K}|)] + \Delta^{\mathbb{M}_1}(\Delta^{\mathbb{M}_1} + 2|\mathbb{M}_{1,NK}|).$$

For the “sophisticated” bound, we refer to [3]. We see that our variance approximations and the corresponding error estimates give in fact sharper bounds. The direct error bound is about 30 times larger, the sophisticated error bound still is about three times larger in average.

Compared to the deterministic problems, the effectivity bound $\eta(\mu, \omega)$ from (3.12) contains an additional factor of the form $(1 + c)/(1 - c)$, where c is given by (3.13). Figure 6.10 shows the average factor, its standard deviation, and 100 random samples for each parameter of the test set. We can see that the additional factor takes an average value of about 1.3. Hence, compared to the deterministic case, the effectivity upper bound increases only moderately.

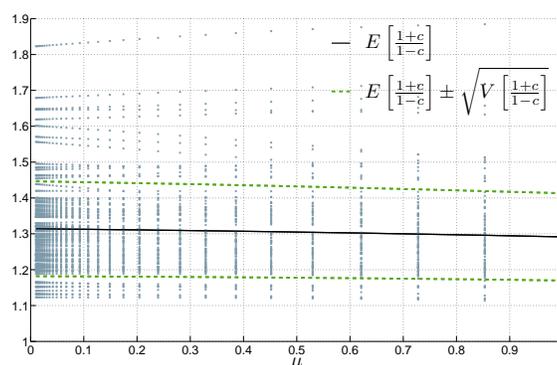


FIGURE 6.10. Mean of effectivity bound factor $\frac{1+c}{1-c}$, its standard deviation, and 100 random samples for a test set of 30 logarithmically distributed values of μ , respectively

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