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# Multi-level Monte Carlo Finite Element method for elliptic PDEs with stochastic coefficients

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**Abstract** In Monte Carlo methods quadrupling the sample size halves the error. In simulations of stochastic partial differential equations (SPDEs), the total work is the sample size times the solution cost of an instance of the partial differential equation. A Multi-level Monte Carlo method is introduced which allows, in certain cases, to reduce the overall work to that of the discretization of one instance of the deterministic PDE. The model problem is an elliptic equation with stochastic coefficients. Multi-level Monte Carlo errors and work estimates are given both for the mean of the solutions and for higher moments. The overall complexity of computing mean fields as well as k-point correlations of the random solution is proved to be of log-linear complexity in the number of unknowns of a single Multi-level solve of the deterministic elliptic problem. Numerical examples complete the theoretical analysis.

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# 1 Introduction

Monte Carlo methods are widely used in statistical simulation. In the case of partial differential equations with random inputs, "sampling" entails the numerical solution of one deterministic partial differential equation (PDE) per sample. For time dependent,

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parabolic problems driven by noise (see, e.g. [3–5,15,22]), numerous paths must be simulated. Here, we are concerned with Monte Carlo methods (MC methods) for elliptic problems where the source of randomness lies in the coefficients. Such problems arise prominently in the numerical simulation of subsurface flow problems (see, e.g. [27,28] and the references therein). Some key characteristics of elliptic problems with stochastic coefficients, which arise in computational geosciences, are the low spatial regularity of the permeability samples, the small spatial correlation lengths (this implies slow convergence of Karhunen–Loève expansions), and, more challenging, the possible non-stationarity of realistic stochastic models. All these factors hinder the efficient numerical simulation of such problems. In order to deal with these difficulties, we propose a Multi-level Monte Carlo method (MLMC method). This family of methods was introduced, to the authors' knowledge, by Giles [17,18] for Itô stochastic ordinary differential equations after earlier work by Heinrich on numerical quadrature (see [21]).

We consider the following elliptic model problem

$$-\operatorname{div}(a\nabla u) = f$$
 in  $D$ ,

where  $D \subset \mathbb{R}^d$ , d = 1, 2, ... We impose mixed Dirichlet and Neumann boundary conditions and assume f to be in  $L^2(D)$ . The coefficient a is assumed to be a possibly correlated random field over the spatial domain D. The random field solution u of Problem (1.1) not only depends on  $x \in \mathbb{R}^d$ , but also on a stochastic parameter  $\omega \in \Omega$ , where  $\Omega$  is the space of all elementary events, which we specify later. For a fixed  $\omega$ , Eq. (1.1) is an elliptic PDE with inhomogeneous coefficient, which can be solved efficiently by a Galerkin Finite Element approximation and Multi-level methods. We shall be interested in particular in the computation of moments of the stochastic solution by a Monte Carlo method (MC method). However, the rate of convergence of the MC method is 1/2, so that quadrupling of the sample size halves the error of the approximation. To estimate the moments of the solution of Eq. (1.1), we must solve the deterministic equation for each sample and form the k-fold tensor product of the Finite Element solution. The cost of this algorithm is the number of samples times the cost for the approximation in the space domain (in the case of a Finite Element method this corresponds to the degrees of freedom).

One of the aims of the Multi-level Monte Carlo Finite Element method (MLMC-FE method), proposed here, is to decrease the cost of this computation to log-linear complexity of N, the number of degrees of freedom of a single deterministic instance of Eq. (1.1) by a Multi-level method, at least for low order Finite Elements. In order to do so, we introduce a nested sequence of hierarchic Finite Element spaces (FE spaces), in each of which we calculate a certain number of samples of the approximation of the solution. As observed initially by Giles in the context of Itô-SDEs in [18], this leads on the one hand to a large number of samples on a very coarse grid, whereas only few samples are needed on a fine grid where the convergence in the space variable x is fast, but solving the linear system of equations for each sample is expensive. Our error analysis shows how the MLMC method exploits this fact: we prove that the optimal number of MC samples is related to an inverse power of the meshwidth at each level of discretization. This strategy provides substantial gains in the efficiency compared

to a MC method. With the use of a full Multigrid solver, the computational cost of the MLMC method is shown to be log-linear in N, the number of degrees of freedom on the finest grid, in  $\mathbb{R}^d$ , for d > 1. Moreover, the error of the MLMC method balances the error of the space approximation and the sampling error. The sample size should therefore be increased if the space approximation is "too good" or the solution "too smooth". Depending on the dimension of the physical domain, the complexity of the MLMC method with linear Finite Elements becomes then, in terms of the number of degrees of freedom, less efficient.

Further we analyze the MLMC approximation of higher moments of the solution. To this end, we propose estimators which are based on sparse tensor products of wavelet representations of the FE solutions for the samples of the random coefficients. This leads to a sparse tensor MLMC-FE method which exhibits near optimal asymptotic error bounds for *k*-point correlations of any order *k*, and, as we show in Sect. 5, is of log-linear complexity in the number *N* of degrees of freedom. As key step in our analysis, we show that the solution exhibits a certain "mix" regularity, which takes the form of *r*-summability of the stochastic solution as a Bochner function in a scale  $\{X_s\}_{s>0}$  of Sobolev spaces on the domain *D*.

This paper is structured as follows. In the second chapter we present all the preliminaries. This is followed by the formulation of our model problem, where we also study the well posedness and certain regularity conditions of the solution. In the fourth chapter we analyze the rate of convergence of the Multi-level Monte Carlo method. We prove convergence rates of the Monte Carlo approximations for the continuous solution and its Galerkin Finite Element approximation. Chapter 5 contains the extension of our previous results to the approximation of higher order moments of the solution. Here we derive rates of convergence for the sparse tensor Multi-level Monte Carlo method for the *k*th moment,  $1 \le k \in \mathbb{N}$ , of the solution. Subsequently we present numerical experiments for some examples in one and two space dimensions.

### **2** Preliminaries

For the variational formulation as well as for our error analysis of the MLMC-FE method for the problem at hand, given by Eq. (1.1), we shall require Bochner spaces of *r*-summable functions in  $D \subset \mathbb{R}^d$ , for d = 1, 2, ... To this end, for any Banach space *B* of real-valued functions on the domain *D* with norm  $\|\cdot\|_B$ , we denote the set of strongly measurable, *r*-summable mappings  $v : \Omega \to B$  by

$$L^{r}(\Omega, \mathcal{A}, \mathbb{P}; B) := \{v : \Omega \to B \mid v \text{ strongly measurable}, \|v\|_{L^{r}(\Omega; B)} < \infty\},\$$

where, for  $0 < r \leq \infty$ ,

$$\|v\|_{L^{r}(\Omega;B)} := \begin{cases} \left( \int_{\Omega} \|v(\omega,\cdot)\|_{B}^{r} d\mathbb{P}(\omega) \right)^{1/r} & \text{if } 0 < r < \infty, \\ esssup_{\omega \in \Omega} \|v(\omega,\cdot)\|_{B} & \text{if } r = \infty. \end{cases}$$

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Here we introduced a probability space  $(\Omega, \mathcal{A}, \mathbb{P})$ , where, as usual,  $\Omega$  denotes a set elementary events,  $\mathcal{A} \subset 2^{\Omega}$  the  $\sigma$ -algebra of all possible events and where  $\mathbb{P} : \mathcal{A} \to [0, 1]$  is a probability measure. Let  $\mathcal{B} \in \mathcal{L}(X, Y)$  denote a continuous linear mapping from X to another separable Hilbert space Y. For a random field  $x \in L^r(\Omega; X)$  this mapping defines a random variable  $y = \mathcal{B}x \in L^r(\Omega; Y)$  and

$$\|\mathcal{B}x\|_{L^r(\Omega;Y)} \le C \|x\|_{L^r(\Omega;X)}.$$

Furthermore, there holds

$$\mathcal{B}\int_{\Omega} x(\omega) \, dP(\omega) = \int_{\Omega} \mathcal{B}x(\omega) \, dP(\omega).$$

We refer to Chapter 1 of [13] for a synopsis of these and further results of Banach space valued random variables.

#### 3 Model elliptic problem with stochastic coefficients

In the bounded Lipschitz domain  $D \subset \mathbb{R}^d$ , d = 1, 2, 3, we consider the elliptic diffusion problem with stochastic diffusion coefficient *a* 

$$-\operatorname{div}(a\nabla u) = f \quad \text{in } D. \tag{3.1}$$

Here,  $f \in L^2(D)$  is a given source term. We assume that the Lipschitz boundary  $\Gamma = \partial D$  is partitioned into a finite union of (d - 1)-dimensional planes, which in turn are grouped into a Dirichlet part  $\Gamma_D$  and a Neumann part  $\Gamma_N$ . We assume in addition that

$$|\Gamma_N| \ge 0 \quad \text{and} \quad |\Gamma_D| > 0. \tag{3.2}$$

Furthermore, the exterior unit normal vector  $\vec{n}$  to  $\Gamma$  exists almost everywhere on  $\Gamma$ . Equation (3.1) is completed by the boundary conditions

$$\gamma_0 u := u|_{\Gamma_D} = 0, \quad \gamma_{1,a} u := (a \, \vec{n} \cdot \nabla u)|_{\Gamma_N} = g,$$
(3.3)

where g is a given normal flux on  $\Gamma_N$  (specific assumptions on g will be given below). In the case of the Laplacean, i.e. when a = 1, we write  $\gamma_1$  in place of  $\gamma_{1,a}$ .

To ensure well-posedness of our problem, we require that the following assumption on the stochastic diffusion coefficient a is fulfilled:

**Assumption 3.1** The stochastic diffusion coefficients  $a(\omega, x)$  in Eq. (3.1), and Eq. (3.3) is assumed to be a strongly measurable mapping from  $\Omega$  into  $L^{\infty}(D)$ .

There exist constants  $0 < a_- < a_+ < \infty$  such that the random coefficient  $a(\omega, x)$  in Eq. (3.1) is uniformly elliptic, i.e. for every  $\omega \in \Omega$  holds<sup>1</sup>

$$0 < a_{-} \le \operatorname{essinf}_{x \in D} a(\omega, x) \le \|a(\omega, \cdot)\|_{L^{\infty}(D)} \le a_{+} < \infty.$$
(3.4)

We remark that for Lipschitz domains D the trace operator  $\gamma_0$  in Eq. (3.3) is welldefined and continuous from  $H^1(D)$  onto  $H^{1/2}(\Gamma_D)$ .

For the normal derivative operator  $\gamma_{1,a}$ , we have

**Lemma 3.2** Under Assumption 3.1, for  $f \in L^2(D)$  and every  $0 < r \le \infty$ , the co-normal derivative operator  $\gamma_{1,a}$  in Eq. (3.3) is a well-defined and surjective linear operator from  $L^r(\Omega; H^{-1}_{\Gamma_D}(D, \Delta))$  onto  $L^r(\Omega; H^{-1/2}(\Gamma_N))$  where

$$H^{1}_{\Gamma_{D}}(D, \Delta) := \{ v \in H^{1}(D) : \gamma_{0}v = 0, \quad \Delta v \in L^{2}(D) \}$$

and  $H^{-1/2}(\Gamma_N) := (H_{00}^{1/2}(\Gamma_D))^*$  (with duality being understood with respect to the "pivot" space  $L^2(\Gamma)$ ; see [24] for the definition of  $H_{00}^{1/2}(\Gamma_D)$ ).

#### 3.1 Variational formulation and well-posedness

To present the variational formulation of Eq. (3.1) we introduce the Hilbert space

$$V = H^{1}_{\Gamma_{D}}(D) = \{ v \in H^{1}(D) : \gamma_{0}v = 0 \}.$$
(3.5)

Due to the assumption  $|\Gamma_D| > 0$ , by the continuity of the trace operator  $\gamma_0$  the space *V* is a closed, linear subspace of  $H^1(D)$  and by the Poincaré inequality the expression

$$V \ni v \to ||v|| := \left( \int_D |\nabla v|^2 \, dx \right)^{1/2}$$

is a norm on V. We identify  $L^2(D)$  with its dual and denote by  $V^*$  the dual of V with respect to the "pivot" space  $L^2(D)$ , i.e. we work in the triplet  $V \subset L^2(D) \simeq L^2(D)^* \subset V^*$ .

To derive the variational formulation of the stochastic elliptic boundary value problem, given by Eqs. (3.1)–(3.3) we fix  $\omega \in \Omega$  for the moment. We then multiply Eq. (3.1) by a test function  $v \in L^2(\Omega; V)$  and integrate by parts in *D* to obtain (for fixed  $\omega \in \Omega$ ) the (formal) integral identity

$$\int_{D} a\nabla v \cdot \nabla u \, dx = \int_{D} f v \, dx + \int_{\Gamma_N} g \gamma_0 v \, ds.$$

<sup>&</sup>lt;sup>1</sup> We assume that the random coefficient *a* is, possibly after modification of a given *a* on a null-set, well-defined and computationally accessible for *every*  $\omega \in \Omega$ .

Taking expectations on both sides of this expression, we arrive at the *weak formulation* of the stochastic elliptic boundary value problem (Eqs. (3.1)–(3.3)): given *a* satisfying Assumption 3.1,  $f \in L^2(\Omega; V^*)$  and  $g \in L^2(\Omega; H^{-1/2}(\Gamma_N))$ , which are mutually independent, find  $u \in L^2(\Omega; V)$  such that

$$B(u, v) = F(v) \quad \forall v \in L^2(\Omega; V),$$
(3.6)

where the bilinear form  $B(\cdot, \cdot) : L^2(\Omega; V) \times L^2(\Omega; V) \to \mathbb{R}$  is given by

$$B(u, v) = \mathbb{E}\left[\int_{D} a(\cdot, x)\nabla u(\cdot, x) \cdot \nabla v(\cdot, x) \, dx\right],$$

and

$$F(v) = \mathbb{E}\left[\int_{D} f(\cdot, x)v(\cdot, x) \, dx\right] + \mathbb{E}\left[\int_{\Gamma_{N}} g\gamma_{0}v(\cdot, x) \, ds_{x}\right],$$

where the 'integrals'  $\int_D f(\cdot, x)v(\cdot, x) dx$  and  $\int_{x \in \Gamma_N} \dots ds_x$  understood as  $L^2(\Omega; V) \times L^2(\Omega; V^*)$  respectively as  $L^2(\Omega; H_{00}^{1/2}(\Gamma_N)) \times L^2(\Omega; H^{-1/2}(\Gamma_N))$  duality pairings obtained by extending the corresponding  $L^2$  inner products by continuity. By the Riesz Representation Theorem there exists a linear operator  $A(\omega) \in \mathcal{L}(V, V^*)$  such that for all  $v, w \in V$ 

$$B(v,w) = {}_{V^*} \langle A(\omega)v,w \rangle_V.$$
(3.7)

**Theorem 3.3** Under Assumption 3.1, for every  $f \in L^2(\Omega; V^*)$  and  $g \in L^2(\Omega; H^{-1/2}(\Gamma_N))$ , the weak formulation, Eq. (3.6), of the stochastic elliptic boundary value problem, given by Eqs. (3.1)–(3.3), admits a unique solution  $u \in L^2(\Omega; V)$ .

*Proof* By Assumption 3.1, we have for every  $v, w \in V$ 

$$|B(v, w)| \le \operatorname{esssup}_{\omega \in \Omega} ||a(\cdot, x)||_{L^{\infty}(D)} ||v||_{L^{2}(\Omega; V)} ||w||_{L^{2}(\Omega; V)} \le a_{+} ||v||_{L^{2}(\Omega; V)} ||w||_{L^{2}(\Omega; V)}$$
(3.8)

and

$$B(v, v) \ge a_{-} \|v\|_{L^{2}(\Omega; V)}^{2}.$$
(3.9)

Moreover, for given  $g \in L^2(\Omega; H^{-1/2}(\Gamma_N))$  and  $f \in L^2(\Omega; V^*)$ , we have by the Cauchy–Schwarz and Poincaré inequalities and the continuity of the trace operator  $\gamma_0$  that for every  $w \in V$ 

$$|F(w)| \le ||f||_{L^{2}(\Omega; V^{*})} ||w||_{L^{2}(\Omega; V)} + ||g||_{L^{2}(\Omega; H^{-1/2}(\Gamma_{N}))} ||\gamma_{0}w||_{L^{2}(\Omega; H^{1/2}(\Gamma_{D}))} \le C(D)(||f||_{L^{2}(\Omega; V^{*})}^{2} + ||g||_{L^{2}(\Omega; H^{-1/2}(\Gamma_{N}))}^{2})^{1/2} ||w||_{L^{2}(\Omega; V)}.$$
(3.10)

The assertion now follows from the Lax-Milgram Lemma.

*Remark 3.4* The variational formulation, Eq. (3.6), requires in Assumption 3.1 only the definition and boundedness of the random coefficient  $a \mathbb{P}$ -a.s.. The (stronger) Assumption 3.1 implies in particular the unique solvability of the stochastic diffusion problem, defined in Eq. (3.1) for *every*  $\omega$ ; this is required for the MLMC-FE simulation. Assumption 3.1 in addition also implies

$$\forall \omega \in \Omega : \|u(\omega, \cdot)\|_{V} \le \frac{1}{a_{-}} \left( \|f(\omega, \cdot)\|_{V^{*}}^{2} + \|g(\omega, \cdot)\|_{H^{-1/2}(\Gamma_{N})}^{2} \right)^{1/2}.$$
(3.11)

#### 3.2 Regularity of Solutions

To ensure local  $H^2(D)$  regularity and the existence of higher moments of the stochastic solution  $u \in L^2(\Omega; V)$  we impose additional assumptions on the data f and g:

Assumption 3.5 We assume that  $f \in L^r(\Omega; L^2(D)), g \in L^r(\Omega; H^{1/2}(\Gamma_N))$ , for some  $2 \le r \le \infty$ , and that the mapping  $\Omega \ni \omega \to a(\omega, \cdot)$  takes values in  $W^{1,\infty}(D)$ for *every*  $\omega \in \Omega$ . Moreover, we assume that the sources of randomness, i.e. a, f and (if  $|\Gamma_N| > 0) g$  are independent and strongly measurable as mappings taking values in the respective Banach spaces  $W^{1,\infty}(D), L^2(D)$  and in  $H^{1/2}(\Gamma_N)$ .

By the usual elliptic regularity theory (see, e.g. [16]), Assumption 3.5 ensures in particular that  $u \in H^2_{loc}(D)$ ,  $\mathbb{P}$ -a.s. We have the following

**Proposition 3.6** Under Assumption 3.5 and by Eq. (3.4), the elliptic problem, given by Eqs. (3.1)–(3.3), admits a unique solution  $u \in L^r(\Omega; W)$ . Here, the space W is defined by

$$W := \{ w \in V : \Delta w \in L^2(D), \ \gamma_0 w = 0, \ \gamma_1 w \in H^{1/2}(\Gamma_N) \},\$$

equipped with the norm  $\|\cdot\|_W$  given by

$$\|w\|_W := \|\Delta w\|_{L^2(D)} + \|w\|_{L^2(D)}$$

*Further, with*  $2 \le r \le \infty$  *as in Assumption* 3.5*, there holds the a priori estimate* 

$$\|u\|_{L^{r}(\Omega;W)} \leq C(a) \left(\|f\|_{L^{r}(\Omega;L^{2}(D))} + \|g\|_{L^{r}(\Omega;H^{1/2}(\Gamma_{N}))}\right).$$
(3.12)

Here, C(a) depends on  $a_-$  and  $a_+$ , resp. on  $||a||_{L^{\infty}(\Omega; W^{1,\infty}(D))}$ .

*Proof* The proof is a consequence of the  $W^{1,\infty}(D)$ -regularity of all realizations of the stochastic coefficient *a* which implies that the stochastic solution  $u \in L^2(\Omega; V)$  satisfies the identity

$$-\Delta u(\omega, \cdot) = \frac{1}{a(\omega, \cdot)} \left( f(\omega, \cdot) + \nabla a(\omega, \cdot) \cdot \nabla u(\omega, \cdot) \right) \text{ in } L^2(D), \quad \forall \omega \in \Omega.$$

Therefore we may estimate for every  $\omega \in \Omega$  with a constant C(a) independent of  $\omega$ 

$$\|\Delta u(\omega, \cdot)\|_{L^{2}(D)} \leq C(a) \left( \|f(\omega, \cdot)\|_{L^{2}(D)} + \|g(\omega, \cdot)\|_{H^{1/2}(\Gamma_{N})} \right).$$

Adding the corresponding  $L^2(D)$  bound [which results from Eq. (3.11) and the Poincaré-inequality], raising both sides of the resulting bound on the  $\|\cdot\|_W$  norm of *u* to the power *r* and taking expectations implies the assertion.

We remark that the space W can be characterized as a weighted Sobolev space with weights vanishing at vertices and (in case d = 3) at edges of the polyhedron D; see, e.g. [20].

In the following section we introduce the Galerkin projections our Finite Element method will be based on. We prove convergence of the resulting discrete problem by a Monte Carlo method, before we proceed with the convergence and a work estimate for the MLMC method for the discrete equation.

#### 4 Multi-level Monte Carlo Finite Element method

A key ingredient in MLMC-FE method are pathwise, *hierarchic* Finite Element discretizations of the stochastic elliptic problem (Eq. (3.1)) which we present next. Followed by an error estimate for the Monte Carlo method of the (non-discrete) solution of the problem at hand. From this result we derive a convergence rate for the MC method of the discrete solution (full tensor MC-FE method) and finally for the Multi-level MC-FE method.

#### 4.1 Mean square stability of the Galerkin projection

The Finite Element method which we consider is based on sequences of regular simplicial meshes of quasi-uniform triangles or tetrahedra  $\{\mathcal{T}_l\}_{l=0}^{\infty}$  of the polygonal respectively polyhedral domain *D*. For any  $l \ge 0$ , we denote the meshwidth of  $\mathcal{T}_l$  by

$$h_l = \max_{K \in \mathcal{T}_l} \{ \operatorname{diam}(K) \} =: \max_{K \in \mathcal{T}_l} \{ h_K \}.$$

We recall (see, e.g. [8,9]) that the nested family  $\{\mathcal{T}_l\}_{l=0}^{\infty}$  of regular, simplicial meshes is called  $\kappa$ -shape regular if and only if there exists a  $\kappa < \infty$  such that  $\kappa := \sup_l \kappa_l =$  $\sup_l \max_{K \in \mathcal{T}_l} \frac{h_K}{\rho_K}$ . Here  $\rho_K$  is the radius of the largest ball that can be inscribed into any  $K \in \mathcal{T}_l$ .

The uniform refinement of the mesh is achieved by regular subdivision. This results in the meshwidth  $h_l = 2^{-l}h_0$ , where  $h_0$  denotes the meshwidth of the coarsest triangulation. The nested family  $\{\mathcal{T}_l\}_{l=0}^{\infty}$  of regular, simplicial triangulations obtained in this way is  $\kappa$ -shape regular, since  $\kappa_l = \kappa_0 = \kappa$ .

For  $p \ge 1$  we define the Finite Element spaces as

$$\mathcal{S}^{p}(D,\mathcal{T}) = \{ v \in H^{1}(D) : v |_{K} \in \mathcal{P}_{p}, \forall K \in \mathcal{T} \},$$

$$(4.1)$$

where we denote by  $\mathcal{P}_p(K) = \operatorname{span}\{x^{\alpha} : |\alpha| \le p\}$  the space of polynomials of total degree  $\le p$  on a set *K*. We also denote by

$$\mathcal{S}^p_{\Gamma_D}(D,\mathcal{T}) = \{ v \in H^1_{\Gamma_D}(D) : v |_K \in \mathcal{P}_p, \ \forall K \in \mathcal{T} \},\$$

the corresponding Finite Element space with essential boundary condition, with  $\Gamma_D$  coinciding with a finite union of boundary edges of  $\mathcal{T}_0$ .

The family of FE spaces that we employ is  $\mathcal{V} = \{\mathcal{S}_{\Gamma_D}^1(D, \mathcal{T}_l)\}_{l=0}^{\infty}$ , which is the family of spaces of continuous, piecewise linear functions on the regular, simplicial triangulation  $\{\mathcal{T}_l\}_{l=0}^{\infty}$  that satisfy the homogeneous essential boundary conditions on the Dirichlet boundary  $\Gamma_D$  (whose closure coincides, by assumption, with the union of all closed edges of elements  $K \in \mathcal{T}_l$  abutting at  $\Gamma_D$ ).

The Galerkin approximation is based on the weak formulation in Eq. (3.6) of the stochastic elliptic boundary value problem, presented in Eqs. (3.1)–(3.3).

Since for each level *l* of mesh refinement,  $V_l = S^1_{\Gamma_D}(D, \mathcal{T}_l) \subset H^1_{\Gamma_D}(D)$  the corresponding discrete problem reads: find  $u_l \in L^2(\Omega; S^1_{\Gamma_D}(D, \mathcal{T}_l))$  such that

$$B(u_l, v_l) = F(v_l) \quad \forall v_l \in L^2(\Omega; \mathcal{S}^1_{\Gamma_D}(D, \mathcal{T}_l)),$$
(4.2)

where F(v) is defined as in Eq. (3.6).

By Eqs. (3.8), (3.9) and (3.10), for each l = 0, 1, 2, ... exists a unique stochastic FE solution  $u_l \in L^2(\Omega; \mathcal{S}^1_{\Gamma_D}(D, \mathcal{T}_l)).$ 

The operator  $G_l$  projecting the variational solution  $u \in L^2(\Omega; V)$  into the stochastic Finite Element solution  $u_l \in L^2(\Omega; S^1_{\Gamma_D}(D, \mathcal{T}_l))$  is an  $L^2(\Omega; V)$ -stable projection: by Eqs. (4.2) and (3.9), we have for every l

$$a_{-} \|u_{l}\|_{L^{2}(\Omega; V)}^{2} \leq B(u_{l}, u_{l}) = B(u, u_{l}) \leq a_{+} \|u\|_{L^{2}(\Omega; V)} \|u_{l}\|_{L^{2}(\Omega; V)},$$

which implies

$$\|G_{l}v\|_{L^{2}(\Omega;V)} \leq \frac{1}{a_{-}} \|v\|_{L^{2}(\Omega;V)} \quad \forall v \in L^{2}(\Omega;V).$$

Under Assumption 3.1, the Galerkin projection  $G_l$  is well-known to be quasioptimal (see, e.g. [8,9]), i.e.

$$\|u - u_l\|_{L^2(\Omega; V)} \le C_a \inf_{v_l \in V_l} \|u - v_l\|_{L^2(\Omega; V)},$$
(4.3)

where  $C_a = \sqrt{\frac{a_+}{a_-}}$ .

Assumptions 3.1 and 3.5 imply local  $H^2(D)$ -regularity of the solution. More precisely, with the space  $W \subset V$  as defined in Eq. (3.12), there exists a unique weak solution  $u \in L^2(\Omega; W)$  and Eq. (3.12) holds. Then, C(a) depends on  $a_-$  and  $a_+$  resp. on  $||a||_{L^{\infty}(\Omega; W^{1,\infty}(D))}$ . With the same assumptions and by well known results (see for example [8,9]) we have for all  $w \in W$  and every  $l \in \mathbb{N}_0$ 

$$\inf_{v_l \in \mathcal{S}^1_{\Gamma_D}(D,\mathcal{T}_l)} \|w - v_l\|_{H^1_{\Gamma_D}(D)} \le C_I 2^{-l} h_0 \|w\|_W,$$
(4.4)

where  $C_I > 0$  is some constant, independent of *l*.

We proceed with an analysis of the rate of convergence of the Monte Carlo method for the solution of the stochastic elliptic problem (3.6). First we derive the estimate for the solution which is not discretized in space and then generalize this result to the Finite Element solution.

#### 4.2 Rate of convergence of the Monte Carlo method

We are interested in estimating statistical moments of the random solution. We estimate the expectation  $\mathbb{E}[u] \in V$  by the mean over solution samples  $\hat{u}^i \in V, i = 1, ..., M$  corresponding to M independent, identically distributed realizations of the random input data a, f and g:

$$E_M[u] := \frac{1}{M} \sum_{i=1}^M \hat{u}^i \in V.$$
(4.5)

The following result is a bound on the *statistical error* resulting from this Monte Carlo estimator.

**Lemma 4.1** For any  $M \in \mathbb{N}$  and for  $u \in L^2(\Omega; V)$  holds

$$\|\mathbb{E}[u] - E_M[u]\|_{L^2(\Omega;V)} \le M^{-1/2} \|u\|_{L^2(\Omega;V)}.$$

*Proof* Let us denote by  $\hat{u}_M$  the sample average over M samples. Defined as such  $\hat{u}_M$  is a random variable that maps  $\Omega$  into V. With the independence of the identically distributed samples it follows

$$\begin{split} \|\mathbb{E}[u] - E_{M}[u]\|_{L^{2}(\Omega;V)}^{2} &= \mathbb{E}\left[\left\|\mathbb{E}[u] - \frac{1}{M}\sum_{i=1}^{M}\hat{u}^{i}\right\|_{V}^{2}\right] = \frac{1}{M^{2}}\sum_{i=1}^{M}\mathbb{E}\left[\left\|\mathbb{E}[u] - \hat{u}^{i}\right\|_{V}^{2}\right] \\ &= \frac{1}{M}\mathbb{E}\left[\left\|\mathbb{E}[u] - u\right\|_{V}^{2}\right] = \frac{1}{M}(\mathbb{E}\|u\|_{V}^{2} - \|\mathbb{E}[u]\|_{V}^{2}) \\ &\leq \frac{1}{M}\|u\|_{L^{2}(\Omega;V)}^{2}. \end{split}$$

4.3 Single-level Monte Carlo Finite Element method

The implementation of the estimator  $E_M[u]$  in Eq. (4.5) requires a Finite Element approximation of the 'samples'  $\hat{u}^i$  which we choose from a continuous, piecewise

linear Finite Element space on a family of shape regular, affine and simplicial triangulations  $\{\mathcal{T}_l\}_{l=0}^{\infty}$ .

The key question which arises naturally here is which is the optimal choice of the sample size in dependence of the grid size to achieve a prescribed error level with minimal work.

We shall address this question under the following assumptions on the Finite Element method.

**Assumption 4.2** For a given Finite Element mesh  $\mathcal{T}_l$  from the family of meshes the FE solution for a given realization  $\hat{a}^i \in W^{1,\infty}(D)$  of the stochastic coefficient which satisfies Assumption 3.1, the Galerkin projection  $u_l = G_l u \in V_l$  on the Finite Element subspace  $V_l = S^1_{\Gamma_D}(D, \mathcal{T}_l)$  of dimension  $N_l = \dim(S^1_{\Gamma_D}(D, \mathcal{T}_l))$  can be realized in  $O(N_l)$  work and memory. The Galerkin projections  $u_l$  admit the a priori error estimate

$$\|w - G_l w\|_V \le C_a C_I h_l \|w\|_W,$$

where  $h_l = 2^{-l} h_0 = \max_{K \in \mathcal{T}_l} \operatorname{diam}(K)$  denotes the meshwidth of  $\mathcal{T}_l$ .

We remark that for polygonal domains  $D \subset \mathbb{R}^2$ , Assumption 4.2 on the space W can be satisfied by standard Multilevel solvers for continuous, piecewise linear Finite Elements on families  $\{\mathcal{T}_l\}_{l=0}^{\infty}$  of meshes with suitable refinement towards the vertices of D. We now establish a first error estimate for the MC-FE method in the case when *the same Finite Element mesh*  $\mathcal{T}_l$  *is used for all samples*: we estimate the expectation of the solution,  $\mathbb{E}[u]$ , by

$$E_{M}[u_{l}] := \frac{1}{M} \sum_{i=1}^{M} G_{l} \hat{u}^{i} \in L^{2}(\Omega; S^{1}(D, \mathcal{T}_{l}))$$
(4.6)

**Theorem 4.3** Under Assumptions 3.1 and 3.5 holds the error bound

$$\|\mathbb{E}[u] - E_M[u_l]\|_{L^2(\Omega; V)} \le C(a) \left(\frac{1}{\sqrt{M}} + h_l\right) \left(\|f\|_{L^2(\Omega; L^2(D))} + \|g\|_{L^2(\Omega; H^{3/2}(\Gamma_N))}\right).$$
(4.7)

*Proof* We split the left hand side of the equation above as follows

$$\begin{aligned} \|\mathbb{E}[u] - E_M[u_l]\|_{L^2(\Omega;V)} &\leq \|\mathbb{E}[u] - \mathbb{E}[u_l]\|_{L^2(\Omega;V)} + \|\mathbb{E}[u_l] - E_M[u_l]\|_{L^2(\Omega;V)} \\ &\leq \mathbb{E}\left[\|[u] - [u_l]\|_V\right] + \|\mathbb{E}[u_l] - E_M[u_l]\|_{L^2(\Omega;V)}. \end{aligned}$$

The first term on the right hand side is bounded by Assumption 4.2 and Proposition 3.6. The assertion follows with Lemma 4.1 for the second term.  $\Box$ 

The optimal choice of sample size versus grid size for a fixed error is reached when the statistical and the discretization errors are equilibrated, i.e. when  $M^{-\frac{1}{2}} = O(h_l) = O(2^{-l})$ . In terms of the degrees of freedom of the Finite Element method,  $N_l$ , therefore, we obtain from Eq. (4.7) the basic relation

$$M^{-\frac{1}{2}} = O(h_l) = O(N_l^{-\frac{1}{d}}).$$
(4.8)

We have a closer look at the computational cost of the Monte Carlo method. We work under Assumption 4.2 and take the same estimate as before, i.e. we estimate  $\mathbb{E}[u]$  by the mean of  $\hat{u}_{l}^{i}$ , i = 1, ..., M for M independent samples with the fixed discretization level l:

$$\mathbb{E}[u_l] \simeq E_M[u_l] = \frac{1}{M} \sum_{i=1}^M \hat{u}_l^i = \frac{1}{M} \sum_{i=1}^M G_l \hat{u}^i.$$

Under Assumption 4.2, the computational cost of this estimate is  $O(M \cdot N_l)$  work and memory, i.e. the number of samples times the cost for each Finite Element solution with  $N_l = 2^{ld}$  degrees of freedom. With the previous calculation on the optimal sample size, i.e. Eq. (4.8), which implies  $M = N_l^{\frac{2}{d}} = O(2^{2l})$ , we may write for the computational cost  $O(2^{l(2+d)})$ .

Subsequently we generalize these calculations to the case of a Multi-level approximation of the Monte Carlo method.

#### 4.4 Multi-level Monte Carlo Finite Element method

For the MLMC method we discretize the variational formulation, given by Eq. (3.6), by Galerkin projection onto the hierarchic sequence  $\mathcal{V}$  of finite dimensional sub-spaces  $V_0(D) \subset V_1(D) \subset \cdots \subset V_l(D) \subset \cdots \subset V(D)$ , where  $V_l(D) := S^1_{\Gamma_D}(D, \mathcal{T}_l)$ . With the notation  $u_0 := 0$  we may write

$$u_L = \sum_{l=1}^{L} (u_l - u_{l-1})$$

and, by linearity of the expectation operator  $\mathbb{E}[\cdot]$ ,

$$\mathbb{E}[u_L] = \mathbb{E}\left[\sum_{l=1}^L (u_l - u_{l-1})\right] = \sum_{l=1}^L \mathbb{E}[u_l - u_{l-1}].$$

In the MLMC-FE method, we estimate  $\mathbb{E}[u_l - u_{l-1}]$  by a level dependent number  $M_l$  of samples, which implies that we may estimate  $\mathbb{E}[u]$  by

$$E^{L}[u] := \sum_{l=1}^{L} E_{M_{l}}[G_{l}u - G_{l-1}u].$$
(4.9)

Convergence of the MLMC-FE method is guaranteed by the following

**Lemma 4.4** Under Assumptions 3.1, 3.5 and 4.2, the MLMC-FE approximation, Eq. (4.9) of the expectation  $\mathbb{E}[u]$  of the solution  $u \in L^2(\Omega; W)$  to the stochastic elliptic boundary value problem, presented in Eqs. (3.1)–(3.3), in the polyhedral domain  $D \subset \mathbb{R}^d$  admits the error bound

$$\|\mathbb{E}[u] - E^{L}[u]\|_{L^{2}(\Omega;V)} \leq C \left(h_{L} + \sum_{l=1}^{L} h_{l} M_{l}^{-1/2}\right) \left(\|f\|_{L^{2}(\Omega;L^{2}(D))} + \|g\|_{L^{2}(\Omega;H^{1/2}(\Gamma_{N}))}\right).$$
(4.10)

Here, the constant C depends only on d,  $a_{-}$  and on the bound  $||a||_{L^{\infty}(\Omega; W^{1,\infty}(D))}$  in Assumption 3.5.

*Proof* We rewrite the error to be estimated as in the proof of Theorem 4.3 as

$$\begin{split} \|\mathbb{E}[u] - E^{L}[u]\|_{L^{2}(\Omega;V)} &= \left\|\mathbb{E}[u] - \mathbb{E}[u_{L}] + \mathbb{E}[u_{L}] - \sum_{l=1}^{L} E_{M_{l}}[u_{l} - u_{l-1}]\right\|_{L^{2}(\Omega;V)} \\ &\leq \|\mathbb{E}[u] - \mathbb{E}[u_{L}]\|_{L^{2}(\Omega;V)} \\ &+ \left\|\sum_{l=1}^{L} \left(\mathbb{E}[u_{l} - u_{l-1}] - E_{M_{l}}[u_{l} - u_{l-1}]\right)\right\|_{L^{2}(\Omega;V)} \\ &=: I + II. \end{split}$$

We estimate the error bounds for the terms *I* and *II* separately.

*Term I*: By Jensen's and the Cauchy–Schwarz inequality, for every l = 1, ..., L, we get

$$I \leq \left( \left[ \|\mathbb{E}(u - G_{l}u)\|_{L^{2}(\Omega; V)}^{2} \right] \right)^{1/2} = \|u - u_{l}\|_{L^{2}(\Omega; V)} \leq C_{I}C_{a}h_{l}\|u\|_{L^{2}(\Omega; W)}.$$

In particular for l = L we obtain the asserted bound for Term *I*.

*Term II*: By the triangle inequality we consider for each l = 1, ..., L the term

$$\|\mathbb{E}[u_l - u_{l-1}] - E_{M_l}[u_l - u_{l-1}]\|_{L^2(\Omega; V)}$$

Each of these terms is estimated as follows:

$$\begin{split} \|\mathbb{E}[u_{l} - u_{l-1}] - E_{M_{l}}[u_{l} - u_{l-1}]\|_{L^{2}(\Omega;V)} &= \|(\mathbb{E} - E_{M_{l}})[u_{l} - u_{l-1}]\|_{L^{2}(\Omega;V)} \\ &\leq M_{l}^{-1/2} \|u_{l} - u_{l-1}\|_{L^{2}(\Omega;V)} \\ &\leq M_{l}^{-1/2} \left(\|u - u_{l}\|_{L^{2}(\Omega;V)} \\ &+ \|u - u_{l-1}\|_{L^{2}(\Omega;V)}\right) \\ &\leq C_{a}C_{I} M_{l}^{-1/2} (h_{l} + h_{l-1})\|u\|_{L^{2}(\Omega;W)} \\ &= 3 C_{a}C_{I} h_{l} M_{l}^{-1/2} \|u\|_{L^{2}(\Omega;W)}. \end{split}$$

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Here we used Lemmas 4.1, Eqs. (4.3) and (4.4). Summing these estimates from l = 1, ..., L completes the proof.

The preceding result gives an error bound for the MLMC-FE approximation, for *any* distribution  $\{M_l\}_{l=1}^{L}$  of samples over the mesh levels. Like in the single-level Monte Carlo approximation one is interested in the optimal ratio of sample size versus grid size in every level, i.e. how  $M_l$  relates to  $h_l$  to achieve an overall convergence rate of  $O(h_L)$ .

**Theorem 4.5** Under Assumptions 3.1, 3.5 and 4.2, the MLMC-FE approximation, given by Eq. (4.9), of the expectation of the solution of the stochastic elliptic boundary value problem (Eqs. (3.1)–(3.3)) in the polyhedral domain  $D \subset \mathbb{R}^d$  with  $M_l$  samples on mesh level l given by  $M_l = O(l^{2+2\epsilon}2^{2(L-l)}h_0), l = 1, 2, ..., L$ , where  $\epsilon > 0$  is arbitrarily small, admits the error bound

$$\|\mathbb{E}[u] - E^{L}[u]\|_{L^{2}(\Omega; V)} \le Ch_{L}(\|f\|_{L^{2}(\Omega; L^{2}(D))} + \|g\|_{L^{2}(\Omega; H^{3/2}(\Gamma_{N}))}).$$

If, at each level l the Finite Element equations for each sample  $\hat{u}_l^i$  in the estimator  $E_{M_l}[u_l]$  are solved approximately with a full Multigrid method to accuracy  $O(h_l)$  in the energy norm, the total work Work(L) and memory for computing  $E^L[u]$  approximately to accuracy  $O(h_L)$  is bounded by

$$Work(L) \le C_{\epsilon} \begin{cases} N_L^2 & \text{for } d = 1, \\ N_L (\log N_L)^{3+\epsilon} & \text{for } d = 2, \\ N_L (\log N_L)^{2+\epsilon} & \text{for } d = 3, \end{cases}$$

where the constant C depends on  $\epsilon$  but is independent of L.

*Proof* The convergence result in Lemma 4.4 suggests that we choose  $M_l$  such that the overall rate of convergence is  $O(h_L)$ . With the choice

$$M_l = \mathcal{O}(l^{2+2\epsilon} (h_l/h_L)^2) = \mathcal{O}(l^{2+2\epsilon} 2^{2(L-l)}), \quad l = 1, \dots, L$$
(4.11)

for some  $\epsilon > 0$ , we obtain from Eq. (4.10) the asserted error bound, since for  $\epsilon > 0$  this implies

$$\sum_{l=1}^{L} h_l M_l^{-1/2} \le C \sum_{l=1}^{L} 2^{-l} h_0 l^{-(1+\epsilon)} 2^{(l-L)} h_0 \le C 2^{-L} h_0 \sum_{l=1}^{L} l^{-(1+\epsilon)}$$
$$\le C h_L \sum_{l=1}^{L} l^{-(1+\epsilon)} = C(\epsilon) h_L.$$

To estimate the work, we observe that the approximate solution given by the Finite Element equation solved by a full Multigrid method at mesh level *l* to accuracy  $h_l$  is of linear complexity in the number  $N_l$  of unknowns at mesh level *l* (see, e.g. [8,9]). For  $M_l$  samples (possibly in parallel) this requires a total of  $O(M_l N_l)$  computational

work and memory. This amounts to the following bound for the overall work for the MLMC-FE method at level L

$$Work(L) \lesssim \sum_{l=1}^{L} M_l N_l \leq \sum_{l=1}^{L} l^{2+2\epsilon} 2^{2(L-l)} 2^{dl}$$
$$= 2^{dL} \sum_{l=1}^{L} l^{2+2\epsilon} 2^{2(L-l)} 2^{d(l-L)} = 2^{dL} \sum_{l=1}^{L} l^{2+2\epsilon} 2^{(d-2)(l-L)}$$
$$\lesssim N_L \begin{cases} \sum_{l'=0}^{L-1} (L-l')^{2+2\epsilon} 2^{l'} & \text{for } d = 1, \\ \sum_{l'=0}^{L-1} (L-l')^{2+2\epsilon} & \text{for } d = 2, \\ \sum_{l'=0}^{L-1} (L-l')^{2+2\epsilon} 2^{-l'} & \text{for } d = 3. \end{cases}$$

This implies the asserted work estimates, if we use in the case d = 1 for  $0 < \epsilon < 1$  summation by parts three times.

*Remark 4.6* We remark that in the particular case d = 1, i.e. when the domain D coincides with an interval, with the standard "hat function" basis for  $S^1(D, T_l)$  the stiffness matrix is tridiagonal and symmetric positive definite provided Assumption 3.1 is satisfied. Therefore, direct solvers are applicable with complexity  $O(N_l)$ .

*Remark 4.7* In the same particular case d = 1, the approximation with standard "hat functions" is already too accurate for the model problem. Since we equilibrate the errors of the MC method and the FE method, the MC error is dominating the overall error, leading to an increase of the samples which causes the quadratic complexity. In the cases of higher space dimensions the accuracy of the FE approximation, expressed in terms of the degrees of freedom, is lower. In this case the overall error is not dominated by the MC error.

In the subsequent chapter we further detail these results for the mean field to the approximation of higher moments of the solution of the elliptic model problem.

#### **5** Multi-level Monte Carlo Finite Element approximation of higher moments

We now address two generalizations of the MLMC-FE approximation: the efficient computation of kth moments of the stochastic solution  $u \in L^2(\Omega; V)$ , and the use of Finite Elements which are based on continuous, piecewise polynomials of degree  $p \ge 1$ . In particular the case k = 2, i.e. second moments, is of substantial interest in practice. Since, however, kth moments (which are sometimes referred to as k-point correlation functions) are functions on the k-fold product domain  $D^k = D \times \cdots \times D$ , a naive MC estimation (with M samples) of the product of the solution vectors will entail complexity  $MN_L^k$ . The main result of the present section states that in order to recover log-linear complexity of kth moments with  $k \ge 2$ , the MLMC-FE approximation must be combined with a wavelet compression of the Finite Element solutions for each sample. For k = 1, the results constitute a generalization of the preceding analysis to higher order elements. For k = 2 in two spatial dimensions (i.e. when d = 2) we obtain in particular a log-linear complexity scheme for the computation of a Galerkin approximation to the so-called "4*d*-VAR" of the stochastic solution.

Therefore, we first establish the regularity of the *k*th moment of the solution of the elliptic problem given certain smoothness and regularity conditions on the data and the coefficient and we introduce wavelet bases for the hierarchical meshes. Under these assumptions we derive full and sparse tensor error bounds for the Finite Element approximation. Those bounds are essential for the error of the sparse tensor MLMC-FE approximation.

#### 5.1 Existence and Regularity of kth Moments

We are interested in statistical moments of the stochastic solution u: for any  $k \in \mathbb{N}$  we denote the *k*-fold tensor products of a separable Hilbert space *X* as

$$X^{(k)} = \underbrace{X \otimes \cdots \otimes X}_{k-\text{times}},$$

equipped with the natural norm  $\|\cdot\|_{X^{(k)}}$ . This norm has the property that for every  $u_1, \ldots, u_k \in X$  there holds the isometry

$$||u_1 \otimes \cdots \otimes u_k||_{X^{(k)}} = ||u_1||_X \cdots ||u_k||_X.$$

For  $u \in L^k(\Omega; X)$  we now consider the random field  $(u)^{(k)}$  defined by  $u(\omega) \otimes \cdots \otimes u(\omega)$ . Then  $(u)^{(k)} = u \otimes \cdots \otimes u \in L^1(\Omega, X^{(k)})$  and we have the isometry

$$\|(u)^{(k)}\|_{L^{1}(\Omega; X^{(k)})} = \int_{\Omega} \|u(\omega) \otimes \cdots \otimes u(\omega)\|_{X^{(k)}} dP(\omega)$$
$$= \int_{\Omega} \|u(\omega)\|_{X}^{k} dP(\omega) = \|u\|_{L^{k}(\Omega; X)}^{k}.$$
(5.1)

Therefore, we define the moment  $\mathcal{M}^k u$  as the expectation of  $(u)^{(k)} = \underbrace{u \otimes \cdots \otimes u}_{k-times}$ :

**Definition 5.1** For  $u \in L^k(\Omega; V)$ , for some integer  $k \ge 1$ , the *k*th moment (or *k*-point correlation function) of  $u(\omega)$  is defined by

$$\mathcal{M}^{k} u = \mathbb{E}[(u)^{(k)}] = \mathbb{E}[\underbrace{u \otimes \cdots \otimes u}_{k-times}]$$
$$= \int_{\omega \in \Omega} \underbrace{u(\omega) \otimes \cdots \otimes u(\omega)}_{k-times} dP(\omega) \in V^{(k)}.$$
(5.2)

As above, the numerical analysis of the higher order MLMC-FE method requires a regularity theory for solutions of Eqs. (3.1)–(3.3). To this end we introduce a

smoothness scale  $(Y_s)_{s\geq 0}$  for the data f, g with  $Y_0 = H^{-1}(D) \times H^{-1/2}(\Gamma_N)$  and with  $Y_s \subset Y_t$  for s > t.

We assume that we have a corresponding scale  $(X_s)_{s\geq 0}$  of "smoothness spaces" for the solutions with  $X_0 = V = H^1_{\Gamma_D}(D)$  and with  $X_s \subset X_t$  for s > t, such that  $(A(\omega))^{-1} \colon Y_s \to X_s$ , defined in Eq. (3.7), is continuous for all coefficient realization  $\mathbb{P}$ -a.s.

For our model problem, Eqs. (3.1)–(3.3) with smooth random coefficients  $a(\omega, x)$ in a domain D with smooth boundary  $\partial D$  and with  $\Gamma_N = \emptyset$ , we may choose  $Y_s = V^* \cap H^{-1+s}(D) \times H^{-1/2+s}(\Gamma_N)$  and  $X_s = V \cap H^{1+s}(D)$  for any s > 0. We remark that in non-smooth domains such as polyhedra in  $\mathbb{R}^3$  the spaces  $X_s$  are weighted spaces which contain functions which are singular at corners and edges (see, e.g. [20]). We can now state our assumptions on the data of the model problem, given by Eqs. (3.1)–(3.3):

Assumption 5.2 For some  $r^* \ge 2$  and some  $s^* > 0$ , the data (f, g) in Problems (3.1)– (3.3) belong to  $L^{r^*}(\Omega; Y_{s^*})$  and the mapping  $\Omega \ni \omega \to a(\omega, \cdot)$  is such that the operator  $A(\omega)$  is boundedly invertible from  $Y_s$  to  $X_s \subset V\mathbb{P}$ -a.s. for all  $0 < s \le s^*$  for some  $s^* > 0$ . Moreover, the random inputs a, f and g are independent.

We remark that Assumption 5.2 is satisfied if  $a(\cdot, \omega) \in W^{s,\infty}(D)$  for  $\mathbb{P}$ -a.e.  $\omega \in \Omega$ and every  $0 \le s \le s^*$ .

**Theorem 5.3** If Assumptions 3.1 and 5.2 hold, then for every  $2 \le k \le r^*$ , for all  $1 \le r \le r^*/k$ , and every  $0 \le s < s^*$  holds the a priori estimate

$$\|(u)^{(k)}\|_{L^{r}(\Omega; X_{s}^{(k)})} \leq C\|(f, g)^{(k)}\|_{L^{r}(\Omega; Y_{s}^{(k)})} \leq C\|(f, g)\|_{L^{rk}(\Omega; Y_{s})}^{k}.$$
(5.3)

*Proof* Under Assumption 5.2, the operator  $A(\omega)^{(k)}$  is boundedly invertible from  $Y_s^{(k)}$  to  $X_s^{(k)}$  for each coefficient realization  $\mathbb{P}$ -a.s.. The stochastic solution satisfies, for  $\omega \in \Omega \mathbb{P}$ -a.s., the a priori estimate

$$\|u(\omega, \cdot)\|_{X_s} \le C(s, \omega)\|(f, g)(\omega, \cdot)\|_{Y_s}, \quad 0 \le s \le s^*,$$

with a random variable  $C(s, \cdot) \in L^{\infty}(\Omega)$ . Raising both sides of the bounds to the *r*th power and integrating the resulting inequality over  $\omega \in \Omega$  with respect to the probability measure  $\mathbb{P}(d\omega)$ , we obtain the first inequality. The second inequality follows from the isometry given in Eq. (5.1).

Note in particular that in the case s = 1, we have  $W = X_1$ ,  $Y_1 = H^{1/2}(\Gamma_N) \times L^2(D)$ and for k = 2 Assumption 3.5 with r = 2 and Eq. (3.12) imply the a priori estimates

$$\begin{split} \|\mathcal{M}^{2}u\|_{W^{(2)}} &= \|\mathbb{E}[(u)^{(2)}]\|_{W^{(2)}} \leq \|u\|_{L^{4}(\Omega;W)}^{2} \\ &\leq C(a) \left( \|f\|_{L^{4}(\Omega;L^{2}(D))}^{2} + \|g\|_{L^{4}(\Omega;H^{1/2}(\Gamma_{N}))}^{2} \right), \end{split}$$

and

$$\|(u)^{(2)}\|_{L^{2}(\Omega; W^{(2)})} \leq C(a) \left( \|f\|_{L^{4}(\Omega; L^{2}(D))}^{2} + \|g\|_{L^{4}(\Omega; H^{1/2}(\Gamma_{N}))}^{2} \right).$$

#### 5.2 Finite elements with uniform mesh refinement

We now generalize the foregoing analysis to subspaces  $V_l$  of simplicial Finite Elements of order  $p \ge 1$ .

Let us first consider the case of a bounded polyhedron  $D \subset \mathbb{R}^d$ . Let  $\{\mathcal{T}_l\}_{l=0}^{\infty}$  be the sequence of partitions obtained by uniform mesh refinement. Then  $V_l = S_{\Gamma_D}^p(D, \mathcal{T}_l)$  with  $h_l = \max\{\operatorname{diam}(K) : K \in \mathcal{T}_l\} = 2^{-l}h_0$ . We obtain  $N_l = \operatorname{dim} V_l = O(h_l^{-d})$ . With *V* as before, and  $X_s = V \cap H^{1+s}(D)$  the standard Finite Element approximation results give that the following bound holds for  $s \in [0, p]$ .

$$\inf_{v \in V_l} \|u - v\|_V \le C N_l^{-s/d} \|u\|_{X_s}.$$
(5.4)

#### 5.3 Wavelet basis for $V_l$

We introduce a hierarchical basis for the nested spaces  $V_0 \subset \cdots \subset V_L$ : we start with a basis  $\{(\psi_l)_j\}_{j=1,...,N_0}$  for the space  $V_0$ . We write the finer spaces  $V_l$  with l > 0 as a direct sum  $V_l = V_{l-1} \oplus W_l$  with a suitable space  $W_l$ . We assume available explicit basis functions  $\{(\psi_l)_j\}_{j=1,...,\bar{N}_l}$ . Therefore we have that  $V_L = V_0 \oplus W_1 \oplus \cdots \oplus W_L$ , and  $\{(\psi_l)_j \mid l = 0, ..., L; j = 1, ..., \bar{N}_l\}$  is a hierarchical basis for  $V_L$  where  $\bar{N}_0 := N_0$ :

(W1) 
$$V_l = \text{span}\{(\psi_l)_j | 1 \le j \le N_k, 0 \le k \le l\},\$$

with  $N_l := \dim V_l$  and,  $\overline{N}_l := N_l - N_{l-1}$  for  $l \ge 0$ .

Property (W1) is in principle sufficient for the formulation and implementation of the sparse MC-FE method and the deterministic sparse Finite Element method. In order to obtain an algorithm with log-linear complexity we will need that the hierarchical basis satisfies the additional properties (W2)–(W6) of a *wavelet basis*. This will allow us to perform matrix compression, and to obtain optimal preconditioning for the iterative linear system solver (Fig. 1).

- (W2) Small support diam  $\operatorname{supp}((\psi_l)_i) = O(2^{-l}).$
- (W3) *Biorthogonal basis* there exists a biorthogonal basis  $\tilde{\Psi} = \{(\tilde{\psi}_l)_j : 1 \le j \le \bar{N}_k, 0 \le k \le l = 1, 2, ...\}$  such that

$$\langle (\psi_l)_{j}, (\tilde{\psi}_{l'})_{j'} \rangle = \delta_{ll'} \delta_{jj'}.$$

(W4) Energy norm stability there is a constant  $C_B > 0$  independent of level L, such that for all  $v_L = \sum_{l=0}^{L} \sum_{j=1}^{\bar{N}_l} (v_l)_j (\psi_l)_j(x) \in V_L$  holds  $(v_l)_j = \langle v, (\psi_l)_j \rangle$  and

$$\frac{1}{C_B} \sum_{l=0}^{L} \sum_{j=1}^{\bar{N}_l} |(v_l)_j|^2 \le ||v_L||_V^2 \le C_B \sum_{l=0}^{L} \sum_{j=1}^{\bar{N}_l} |(v_l)_j|^2.$$

(W5) Wavelets  $(\psi_l)_i$  with  $l \ge l_0$  have vanishing moments up to order  $p_0 \ge p-2$ 

$$\int (\psi_l)_j(x) \, x^{\alpha} \, dx = 0, \quad 0 \le |\alpha| \le p_0.$$

Except possibly for wavelets where the closure of the support intersects the boundary  $\partial D$  or the boundaries of the coarsest mesh.

(W6) Decay of coefficients for "smooth" functions in  $X_s$  there exists C > 0 independent of L such that for every  $v \in X_s$  and every L holds

$$\sum_{l=0}^{L} \sum_{j=1}^{\bar{N}_{l}} |(v_{l})_{j}|^{2} 2^{2ls} \leq CL^{\nu} ||v||_{X_{s}}^{2},$$
$$\nu = \begin{cases} 0 & \text{for } 0 \leq s < p, \\ 1 & \text{for } s = p. \end{cases}$$

Piecewise polynomial, Finite Element wavelet bases satisfying (W1)–(W6) are available, also in polygonal and polyhedral domains *D*. Any function  $u \in V$  admits a wavelet expansion  $\sum_{l=0}^{\infty} \sum_{j=1}^{\tilde{N}_l} (u_l)_j (\psi_l)_j$ . We define the projection  $P_L : V \to V_L$  by truncating this wavelet expansion of *u*, i.e.

$$P_L u := \sum_{\ell=0}^L \sum_{j=1}^{\bar{N}_l} (u_l)_j (\psi_l)_j, \quad (u_l)_j = \langle u, (\tilde{\psi}_l)_j \rangle.$$

With the stability (W3) and the approximation property in Eq. (5.4) we obtain that the wavelet projection  $P_L$  is quasioptimal: with  $N_L = \dim V_L$ , we have for  $0 \le s \le s^*$  and  $u \in X_s$  the asymptotic error bound

$$||u - P_L u||_V \le C N_L^{-s/d} ||u||_{X_s}.$$

5.4 Full and sparse tensor product spaces

To compute MLMC-FE approximations for  $\mathcal{M}^k u \in V \otimes \cdots \otimes V = V^{(k)}$  (cf. Eq. (5.2)), we project  $\mathcal{M}^k u$  onto a finite dimensional subspace of  $V^{(k)}$ . The choice of the *k*-fold tensor product space  $V_L^{(k)} = V_L \otimes \cdots \otimes V_L$  leads to the *full tensor MC-FE estimates* for  $\mathcal{M}^k u$  in Eq. (5.2):

$$E_M[(u_l)^{(k)}] = \frac{1}{M} \sum_{i=1}^M (\hat{u}_l^i)^{(k)}.$$
(5.5)

Here, the  $\hat{u}_l^i \in V_l$  are the previously discussed Galerkin approximations for  $i = 1, ..., M_l$  i.i.d. samples of the stochastic coefficients.



Fig. 1 Biorthogonal, piecewise linear spline wavelets

The space  $V_L^{(k)}$  has dimension  $N_L^k$  and even forming one tensor product  $(\hat{u}_L^j)^{(k)}$  of a Finite Element sample in the Monte Carlo estimate of Eq. (5.5) would destroy the linear complexity of the MC-FE estimator for moments of order k > 1.

A reduction in cost at, as we shall show, essentially no loss in accuracy, is possible by using so-called sparse tensor products of the Finite Element spaces  $V_l$  which we define next.

We now define the k-fold sparse tensor product space  $\hat{V}_{I}^{(k)}$  by

$$\hat{V}_{L}^{(k)} = \sum_{\substack{\vec{\ell} \in \mathbb{N}_{0}^{k} \\ |\vec{\ell}| \leq L}} V_{\ell_{1}} \otimes \dots \otimes V_{\ell_{k}},$$

where we denote by  $\vec{\ell}$  the vector  $(\ell_1, \ldots, \ell_k) \in \mathbb{N}_0^k$  of discretization levels and its length by  $|\vec{\ell}| = \ell_1 + \cdots + \ell_k$ . We can write *V* as a direct sum by using the complement spaces  $\mathcal{W}_l$ :

$$\hat{V}_{L}^{(k)} = \sum_{\substack{\vec{\ell} \in \mathbb{N}_{0}^{k} \\ |\vec{\ell}| \leq L}} \mathcal{W}_{\ell_{1}} \otimes \cdots \otimes \mathcal{W}_{\ell_{k}}.$$

We define a projection operator  $\widehat{P}_L^{(k)}: V^{(k)} \to \widehat{V}_L^{(k)}$ , for  $x = (x_1, \dots, x_k) \in D^{(k)}$  by truncating the wavelet expansion:

$$(\widehat{P}_{L}^{(k)}v)(x) := \sum_{\substack{0 \le \ell_{1} + \dots + \ell_{k} \le L\\ 1 \le j_{\nu} \le \bar{N}_{\ell_{\nu}}, \nu = 1, \dots, k}} (v_{\ell_{1}\dots\ell_{k}})_{j_{1}\dots j_{k}}(\psi_{\ell_{1}})_{j_{1}}(x_{1})\dots(\psi_{\ell_{k}})_{j_{k}}(x_{k}).$$
(5.6)

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Here, the coefficients are given by

$$(v_{\ell_1\ldots\ell_k})_{j_1\ldots j_k} = {}_{V^{(k)}} \langle v, (\psi_{\ell_1})_{j_1} \otimes \cdots \otimes (\psi_{\ell_k})_{j_k} \rangle_{(V^{(k)})'}.$$

With the projections  $\Pi_l := P_l - P_{l-1}, l = 0, 1, \dots$  and  $P_{-1} := 0$  we can express  $\widehat{P}_L^{(k)}$  as

$$\widehat{P}_L^{(k)} = \sum_{0 \le \ell_1 + \dots + \ell_k \le L} \Pi_{\ell_1} \otimes \dots \otimes \Pi_{\ell_k}.$$

The approximation property of sparse tensor products of the Finite Element spaces, i.e. of  $\hat{V}_{L}^{(k)}$ , was established for example in [19; 31; 32, Proposition 4.2; 34].

**Proposition 5.4** For  $u \in X_s^{(k)}$  with  $0 \le s \le s^*$  we have

$$\inf_{v \in \widehat{V}_L^{(k)}} \|u - v\|_{V^{(k)}} \le C(k) \begin{cases} N_L^{-s/d} \|u\|_{X_s^{(k)}} & \text{if } 0 \le s < p, \\ N_L^{-s/d} L^{(k-1)/2} \|u\|_{X_s^{(k)}} & \text{if } s = p. \end{cases}$$

The stability property (W3) implies the following result (see, e.g. [34]):

**Lemma 5.5** (Properties of  $\widehat{P}_L^{(k)}$ ) Assume (W1)–(W6) and that the component spaces  $V_{\ell}$  of  $\widehat{V}_L^{(k)}$  have the approximation property given in Eq. (5.4). Then for  $u \in V^{(k)}$  the truncated tensorized wavelet expansion is stable, i.e. for every  $k \in \mathbb{N}$  exists C(k) > 0 such that for every  $u \in V^{(k)}$  and every L holds

$$\|\widehat{P}_{L}^{(k)}u\|_{V^{(k)}} \le C(k) \|u\|_{V^{(k)}}.$$
(5.7)

For  $u \in X_s^{(k)}$  and  $0 \le s \le s^*$  we have quasioptimal convergence of  $\widehat{P}_L^{(k)}u$ :

$$\|u - \widehat{P}_{L}^{(k)}u\|_{V^{(k)}} \le C(k) N_{L}^{-s/d} (\log N_{L})^{(k-1)/2} \|u\|_{X_{s}^{(k)}}.$$
(5.8)

These results provide us with the necessary tools to estimate the rate of convergence for the sparse tensor MLMC-FE method for  $\mathcal{M}^k u$ .

5.5 Sparse tensor Multi-level Monte Carlo approximation of higher moments

We aim at estimating

$$\mathcal{M}^{k} u = \mathbb{E}[(u)^{(k)}] = \mathbb{E}[u \otimes \cdots \otimes u].$$

To do so, we have at our disposal coefficient samples  $a(\omega_i, x)$  and the corresponding Galerkin Finite Element approximations  $u_l(x)$  defined in Eq. (4.2). We therefore

define MLMC-FE estimates as statistical averages of the compressed tensor products of the Galerkin Finite Element approximations as follows:

$$\widehat{E}^{L}[(u_{L})^{(k)}] := \sum_{l=1}^{L} E_{M_{l}} \left[ \widehat{P}_{l}^{(k)}(u_{l})^{(k)} - \widehat{P}_{l-1}^{(k)}(u_{l-1})^{(k)} \right],$$
(5.9)

where we once again used the convention that  $u_0 := 0$  and that  $\widehat{P}_0^{(k)} := 0$ . We remark that due to  $\widehat{P}_l^{(1)} = P_l$ , the estimator in Eq. (5.9) will coincide with our standard MLMC-FE estimator in the case k = 1, i.e. for estimating the expectation of u. We can now state our MLMC-FE error bound for moments  $\mathcal{M}^k u$  of order  $k \ge 2$ .

**Theorem 5.6** Assume that  $(f, g) \in L^{2k}(\Omega, Y_s)$  and that the operators  $A(\omega) \in \mathcal{L}(X_s, Y_s)$ , as defined in (3.7), are boundedly invertible for  $0 \le s \le s^* \mathbb{P}$ -a.s., and that the Finite Element spaces  $S^{p,n}(D, \tau_l)$ , for l = 1, ..., L, defined in Eq. (4.1), satisfy the approximation property in Eq. (5.4).

Then there holds for  $0 \le s \le \min(s^*, p)$  and for any numbers  $M_l$  of coefficient samples in the Galerkin Finite Element method on mesh  $T_l$  the bound

$$\left\|\mathcal{M}^{k}u - \widehat{E}^{L}[(u_{L})^{(k)}]\right\|_{L^{2}(\Omega; V^{(k)})} \lesssim \left(\sum_{l=1}^{L} M_{l}^{-1/2} h_{l}^{s} |\log h_{l}|^{(k-1)/2}\right) \|(f, g)\|_{L^{2k}(\Omega; Y_{s})}^{k}.$$

Here,  $M_L = 1$  and the constant in  $\leq$  depends on *s*, *p*, *k* but is independent of the number *L* of mesh refinements and of the distribution of the numbers  $M_l$  of samples at mesh levels *l*.

Proof We write

$$\begin{split} \|\mathcal{M}^{k}u - \widehat{E}^{L}[(u_{L})^{(k)}]\|_{L^{2}(\Omega; V^{(k)})} &= \|\mathbb{E}[(u)^{(k)}] - \widehat{E}^{L}[(u_{L})^{(k)}]\|_{L^{2}(\Omega; V^{(k)})} \\ &\leq \|\mathbb{E}[(u)^{(k)}] - \mathbb{E}[\widehat{P}_{L}^{(k)}(u_{L})^{(k)}]\|_{L^{2}(\Omega; V^{(k)})} \\ &+ \|\mathbb{E}[\widehat{P}_{L}^{(k)}(u_{L})^{(k)}] - \sum_{l=1}^{L} E_{M_{l}}[\widehat{P}_{l}^{(k)}(u_{l})^{(k)} - \widehat{P}_{l-1}^{(k)}(u_{l-1})^{(k)}]\|_{L^{2}(\Omega; V^{(k)})} \\ &=: I + II. \end{split}$$

We estimate the terms separately. For term *I*, we obtain with Jensen's inequality and Eq. (5.7), for any  $0 \le s \le \min(p, s^*)$ , the error bound

$$I = \left\| \mathbb{E}[(u)^{(k)}] - \mathbb{E}[\widehat{P}_{L}^{(k)}(u_{L})^{(k)}] \right\|_{L^{2}(\Omega; V^{(k)})}$$
  

$$= \left\| \mathbb{E}[(u)^{(k)} - \widehat{P}_{L}^{(k)}(u_{L})^{(k)}] \right\|_{V^{(k)}}$$
  

$$\leq \left\| (u)^{(k)} - \widehat{P}_{L}^{(k)}(u)^{(k)} \right\|_{L^{1}(\Omega; V^{(k)})} + \left\| \widehat{P}_{L}^{(k)}((u)^{(k)} - (u_{L})^{(k)}) \right\|_{L^{1}(\Omega; V^{(k)})}$$
  

$$\lesssim \left\| (I - \widehat{P}_{L}^{(k)})(u)^{(k)} \right\|_{L^{1}(\Omega; V^{(k)})} + \left\| (u)^{(k)} - (u_{L})^{(k)} \right\|_{L^{1}(\Omega; V^{(k)})}$$
  

$$=: I_{a} + I_{b}.$$

Term  $I_a$  is a consistency error which is bounded with Eq. (5.8). To estimate term  $I_b$ , we denote the *k* dependence of this term by  $I_b(k)$ , then we write

$$\begin{split} I_{b}(k) &= \|(u)^{(k)} - (u_{L})^{(k)}\|_{L^{1}(\Omega; V^{(k)})} \\ &\leq \|(u - u_{L}) \otimes (u)^{(k-1)}\|_{L^{1}(\Omega; V^{(k)})} + \|u_{L} \otimes ((u)^{(k-1)} - (u_{L})^{(k-1)})\|_{L^{1}(\Omega; V^{(k)})} \\ &\leq \|u - u_{L}\|_{L^{2}(\Omega; V)}\|(u)^{(k-1)}\|_{L^{2}(\Omega; V^{(k-1)})} \\ &+ \|u_{L}\|_{L^{\infty}(\Omega; V)}\|(u)^{(k-1)} - (u_{L})^{(k-1)}\|_{L^{1}(\Omega; V^{(k-1)})} \\ &= \|u - u_{L}\|_{L^{2}(\Omega; V)}\|u\|_{L^{2k-2}(\Omega; V)}^{k-1} + \|u_{L}\|_{L^{\infty}(\Omega; V)}I_{b}(k-1) \\ &\leq C(s)N_{L}^{-s/d}\|f\|_{L^{2}(\Omega; Y_{s})}\|f\|_{L^{2k-2}(\Omega; V^{*})}^{k-1} + C(a)I_{b}(k-1) \;. \end{split}$$

Induction with respect to k leads to the overall bound for I

$$I \le I_a + I_b(k) \le C(a, f, k) N_L^{-s/d} (\log N_L)^{(k-1)/2}$$

We estimate term *II* as follows.

$$\begin{split} II &= \|\mathbb{E}[\widehat{P}_{L}^{(k)}(u_{L})^{(k)}] - \sum_{l=1}^{L} E_{M_{l}}[\widehat{P}_{l}^{(k)}(u_{l})^{(k)} - \widehat{P}_{l-1}^{(k)}(u_{l-1})^{(k)}]\|_{L^{2}(\Omega;V^{(k)})} \\ &= \left\|\sum_{l=1}^{L} \left\{ (\mathbb{E} - E_{M_{l}})[\widehat{P}_{l}^{(k)}(u_{l})^{(k)} - \widehat{P}_{l-1}^{(k)}(u_{l-1})^{(k)}] \right\} \right\|_{L^{2}(\Omega;V^{(k)})} \\ &\leq \sum_{l=1}^{L} M_{l}^{-1/2} \left\| \widehat{P}_{l}^{(k)}(u_{l})^{(k)} - \widehat{P}_{l-1}^{(k)}(u_{l-1})^{(k)} \right\|_{L^{2}(\Omega;V^{(k)})} \\ &\leq \sum_{l=1}^{L} M_{l}^{-1/2} \left\{ \left\| (u)^{(k)} - \widehat{P}_{l}^{(k)}(u_{l})^{(k)} \right\|_{L^{2}(\Omega;V^{(k)})} \\ &+ \left\| (u)^{(k)} - \widehat{P}_{l-1}^{(k)}(u_{l-1})^{(k)} \right\|_{L^{2}(\Omega;V^{(k)})} \right\} \\ &=: \sum_{l=1}^{L} M_{l}^{-1/2} (III(l) + III(l-1)). \end{split}$$

Each of the terms in the sum is bounded as

$$III(l) := \left\| (u)^{(k)} - \widehat{P}_{l}^{(k)}(u)_{l}^{(k)} \right\|_{L^{2}(\Omega; V^{(k)})} \\ \leq \left\| (u)^{(k)} - \widehat{P}_{l}^{(k)}(u)^{(k)} \right\|_{L^{2}(\Omega; V^{(k)})} + \left\| \widehat{P}_{l}^{(k)}((u)^{(k)} - (u_{l})^{(k)}) \right\|_{L^{2}(\Omega; V^{(k)})} \\ \lesssim \left\| (u)^{(k)} - \widehat{P}_{l}^{(k)}(u)^{(k)} \right\|_{L^{2}(\Omega; V^{(k)})} + \left\| (u)^{(k)} - (u_{l})^{(k)} \right\|_{L^{2}(\Omega; V^{(k)})} \\ =: III_{a} + III_{b}.$$

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We estimate  $III_a$  with Eq. (5.8). Term  $III_b$  is bounded as term  $I_b(k)$ , with l in place of L. Combining the bounds for  $III_a$  and  $III_b$ , we obtain with  $h_l \simeq N_l^{-1/d}$  for every  $k \ge 1$  and every  $l \ge 0$  the error estimate

$$III \leq C(k)N_{l}^{-\min(s,p)/d} (\log N_{l})^{(k-1)/2} ||(u)^{(k)}||_{L^{2}(\Omega; X_{s}^{(k)})} + h_{l}^{k\min(s,p)} ||u||_{L^{2k}(\Omega; X_{s})}^{k}$$
  
$$\leq C(k,s)N_{l}^{-\min(s,p)/d} (\log N_{l})^{(k-1)/2} ||u||_{L^{2k}(\Omega; X_{s})}^{k}$$
  
$$= C(k,s)h_{l}^{\min(s,p)} |\log h_{l}|^{(k-1)/2} ||u||_{L^{2k}(\Omega; X_{s})}^{k}.$$

Using this estimate for each l = 0, ..., L to bound *II*, and referring to Eq. (5.3) with p = 2, we obtain with the estimate for *I* the asserted error bound.

We observe that in the case k = 1 and p = 1, with the choices  $X_0 = V$  and  $X_1 = W$ , we recover the previous results. We now optimize the selection of MC samples  $\{M_l\}_{l=0}^{L}$  and state the resulting overall convergence rate of the MLMC-FE method for moments,  $\mathcal{M}^k u$ , for any order  $k \ge 1$ .

**Theorem 5.7** Assume that  $(f, g) \in L^{2k}(\Omega, Y_s)$  and that the operators  $A(\omega) \in \mathcal{L}(X_s, Y_s)$  are boundedly invertible, for  $0 \leq s \leq \min(s^*, p)$  for  $\omega \in \Omega, \mathbb{P}$ -a.s.

Given any  $k \in \mathbb{N}$ , we choose the number of MC samples in the MC-FE method at level l used in the computation of the MLMC-FE estimators in Eq. (5.9) as

$$M_l = \mathcal{O}(2^{2s(L-l)}(l/L)^{k-1}), \quad l = 1, \dots, L.$$
 (5.10)

Then there holds for  $0 \le s \le \min(s^*, p)$  the error bound

$$\|\mathcal{M}^{k}u - \widehat{E}^{L}[(u_{L})^{(k)}]\|_{L^{2}(\Omega; V^{(k)})} \lesssim h_{L}^{s} |\log h_{L}|^{(k+1)/2} \|(f, g)\|_{L^{2k}(\Omega; Y_{s})}^{k}$$

and the total work  $\widehat{W}(L)$  for computing the MLMC-FE estimator in Eq. (5.9) is bounded by

$$\widehat{W}(L) \le C(k) \begin{cases} N_L (\log N_L)^{k-1} & 2s \le d, \\ N_L^{2s/d} (\log N_L)^{k-1} & 2s > d. \end{cases}$$
(5.11)

*Proof* In Theorem 5.6, we choose the numbers  $M_l$  of samples at mesh level l such that the error contributions from the levels to the error bound are equilibrated. This gives, for l = 1, 2, ..., L,

$$M_l^{-1/2} = 2^{-s(L-l)} (L/l)^{(k-1)/2},$$

which implies Eq. (5.10). Inserting this into the error bound of Theorem 5.6, we obtain Eq. (5.11).

To estimate the complexity, we observe that the work to solve the Galerkin Finite Element equations to the required accuracy  $\mathcal{O}(h_l^s)$  in the  $\|\cdot\|_V$ -norm can be achieved in linear complexity, i.e. in  $\mathcal{O}(N_l) = \mathcal{O}(2^{ld})$  work and memory; this complexity estimate can be attained in two ways: either by using the standard (one-scale) Finite

Element basis and full Multigrid (see e.g. [8,9]), or by using a diagonally preconditioned Richardson iteration in wavelet bases. In the latter case, the wavelet Galerkin Finite Element solution vector is directly obtained in the wavelet representation, so that the formation of the sparse tensor approximation in Eq. (5.6) of the *k*th moment of the Galerkin Finite Element approximation is obtained at cost  $\mathcal{O}(N_l(\log N_l)^{k-1})$ work and memory.

In case the Finite Element solution is computed in the standard (one-scale) basis, the solution vector for each sample must first be transformed into the wavelet basis. This is achieved as usual in  $\mathcal{O}(N_l)$  work and memory by the pyramid scheme (see e.g. [10]). Then the formation of the *k*-fold sparse tensor product of  $\widehat{P}_l u_l^{(k)}$  proceeds again according to Eq. (5.6).

For the work estimate, we therefore obtain

$$\begin{split} \widehat{W}(L) &= \sum_{l=1}^{L} M_l N_l (\log N_l)^{k-1} \\ &\lesssim \sum_{l=1}^{L} 2^{2s(L-l)} (l/L)^{k-1} 2^{dl} l^{k-1} \\ &= 2^{dL} \sum_{l=1}^{L} L^{-(k-1)} l^{2(k-1)} 2^{2sL+l(d-2s)-dL} \\ &= N_L L^{-(k-1)} \sum_{l=1}^{L} l^{2(k-1)} 2^{(l-L)(d-2s)} \\ &= N_L L^{-(k-1)} \sum_{l'=0}^{L-1} (L-l')^{2(k-1)} 2^{l'(2s-d)} \\ &\lesssim N_L L^{-(k-1)} \begin{cases} L^{2(k-1)} & 2s \leq d, \\ \sum_{l'=0}^{L-1} (L-l')^{2(k-1)} 2^{l'(2s-d)} & 2s > d. \end{cases}$$

*Remark* 5.8 We remark that the case discussed in Theorem 4.5 corresponds to the case k = 1, s = 1 and p = 1 in Theorems 5.6 and 5.7. Upon comparing both error bounds and the corresponding work estimates, we observe slight differences in the logarithmic terms; this is due to the slightly more conservative choice of the sample sizes  $M_l$  in Eq. (4.11) which we made in order to avoid the appearance of  $\log h_L$  terms in the error bound of Eq. (4.10). For moments of order  $k \ge 2$ , however, such terms appear in any case due to the sparse tensor approximation error bound in Proposition 5.4 which is sharp, so that the slightly more straightforward selection in Eq. (5.10) is sufficient to achieve the expected convergence rates.

*Remark 5.9* The complexity bound in Eq. (5.11) in Theorem 5.7 indicates loss of log-linear complexity as soon as 2s > d. In this case, the smoothness *s* of the solution mapping  $A(\omega)^{-1}$  allows for higher convergence rates of the Galer-

kin Finite Element approximation in D which, when combined with a linear complexity solver such as Multigrid or a diagonally preconditioned wavelet solver, will imply that the efficiency of the MLMC-FE method (i.e. accuracy versus work) is dominated by the "weaker" of the two methods. In the case s > d/2, this is the MC method. We conclude from Theorem 5.7 that, therefore, the use of a MLMC-FE method is only advisable in connection with low order Finite Element methods: in spatial dimension d = 2, log-linear complexity will be retained with linear simplicial Finite Element methods where p = 1. In spatial dimension d = 3, linear complexity can be retained up to s = 3/2; to access this range of convergence orders, it will suffice to use simplicial Finite Element methods of polynomial degree p = 2. Then, convergence for the expectation and for moments of order  $k \ge 2$  can be achieved with sparse tensor products of the FE solution samples in overall complexity of  $\mathcal{O}(N_L^{4/3}(\log N_L)^{k-1})$  for work and  $\mathcal{O}(N_L(\log N_L)^{k-1})$  for memory.

#### 6 Implementation and examples

In this section we discuss the approximation of the stochastic coefficient *a* for  $\omega \in \Omega$ , followed by numerical examples in  $\mathbb{R}$  and  $\mathbb{R}^2$ .

#### 6.1 Coefficient representations

For numerical simulations, the random field  $a(\omega, x)$  in Eq. (3.1) must be represented parametrically. Here, we discuss the implementation and the complexity of two choices: a Karhunen–Loève expansion and a (multi)wavelet expansion of  $a(\omega, x)$ .

#### 6.1.1 Karhunen-Loève -expansion

Random diffusion coefficients  $a(\omega, x) \in L^2(\Omega; L^2(D))$ , admit a Karhunen–Loève expansion in terms of the eigenpairs  $(\lambda_k, \varphi_k)_{k=1}^{\infty}$  of the covariance operator which is the compact and self-adjoint integral operator with kernel  $q_a$  given by

$$q_a := \mathbb{E}[(a - \mathbb{E}[a]) \otimes (a - \mathbb{E}[a])]$$
(6.1)

or defined pointwise formally by

$$q_a(x, x') := \mathbb{E}[(a(\cdot, x) - \mathbb{E}[a](x))(a(\cdot, x') - \mathbb{E}[a](x'))], \quad x, x' \in D.$$
(6.2)

We assume that the eigenfunctions  $\varphi_k$  are normalized in  $L^2(D)$  and the  $\lambda_k$  are enumerated in decreasing magnitude, then the random diffusion coefficient admits the Karhunen–Loève expansion

$$a(\omega, x) = \mathbb{E}[a](x) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} Y_i(\omega) \varphi_i(x), \qquad (6.3)$$

where the random coefficients  $Y_i(\omega)$ , for i = 1, 2, ..., are defined by

$$Y_{i}(\omega) = \begin{cases} \frac{1}{\sqrt{\lambda_{i}}} \int_{D} (a(\omega, x) - \mathbb{E}[a](x))\varphi_{i}(x) \, dx, & \text{if } \lambda_{i} > 0, \\ 0, & \text{otherwise.} \end{cases}$$
(6.4)

The Karhunen–Loève series in Eq. (6.3) converges in  $L^2(\Omega; L^2(D))$  (see e.g. [33]).

Estimation of the probability density function for the stochastic coefficients  $Y_k$ in the Karhunen–Loève expansion, Eq. (6.3), from an ensemble  $\{\hat{a}^i \in L^{\infty}(D) : i = 1, ..., I\}$ , can be performed via Eq. (6.4) *provided* the Covariance  $Q_a(x, x')$  in Eq. (6.2) is known. In this case, the smoothness of the covariance kernel  $q_a(x, x')$  is well known to determine the rate of decay of the eigenvalues to zero in the Karhunen–Loève expansion (e.g. [33]). Moreover, approximate eigenpairs can be computed via variational methods using Finite Element subspaces, and rates of pointwise convergence in D can be established almost surely. We emphasize that to determine the Karhunen–Loève expansion of the stochastic coefficient a explicit knowledge of the covariance kernel  $q_a$  in Eqs. (6.1) and (6.2) is required.

#### 6.1.2 Wavelet-expansion

The Finite Element spaces  $V_l = S_{\Gamma_D}^1(D, \mathcal{T}_l)$ , as defined in Eq. (4.1), in the domain D are built on the nested sequence  $\{\mathcal{T}_l\}_{l=0}^{\infty}$  of regular, simplicial triangulations  $\tau_l$ , obtained by l uniform refinements of some initial, regular partition  $\mathcal{T}_0$  of D into simplices  $(K_0)_j$ ,  $j = 1, \ldots, \#\mathcal{T}_0$ . Therefore, for each  $l \in \mathbb{N}_0$ , every simplex  $(K_l)_j \in \mathcal{T}_l$  is affinely equivalent to the reference simplex  $\hat{K} = \{\hat{x} \in \mathbb{R}^d_+ : \|\hat{x}\|_1 < 1\}$ : there are affine mappings

$$(F_l)_j : \hat{K} \ni \hat{x} \to x \in (K_l)_j \in \mathcal{T}_l,$$

such that, for all  $j = 1, \ldots, #(T_l)$ ,

$$\det |D(F_l)_j| = |(K_l)_j| / |\hat{K}| = \mathcal{O}(2^{-ld}).$$

We observe that for every  $p \ge 1$  and any regular, simplicial partition  $\mathcal{T}$  of D holds

$$\nabla(\mathcal{S}^{p,1}_{\Gamma_D}(D,\mathcal{T})) \subseteq \mathcal{S}^{p-1,0}(D,\mathcal{T})^d \subset L^2(D)^d.$$
(6.5)

For any  $L, q \in \mathbb{N}_0$ , we have the orthonormal decomposition

$$\mathcal{S}^{q,0}(D,\mathcal{T}_L) = \bigoplus_{l=0}^L R_l,$$

where

$$R_l := S^{q,0}(D, \mathcal{T}_l) \cap S^{q,0}(D, \mathcal{T}_{l-1})^{\perp}$$
 if  $l \ge 1$ , and  $R_0 := S^{q,0}(D, \mathcal{T}_0)$ .

An  $L^2(D)$ -orthonormal basis of  $S^{q,0}(D, \mathcal{T})$  can be explicitly constructed as follows: let  $\hat{\mathcal{T}}_0 = \{\hat{K}\}$  and define  $\hat{\mathcal{T}}_1 = \{(\hat{K}_1)_j : j = 1, ..., 2^d\}$ , the set of  $2^d$  many simplices  $(\hat{K}_1)_j$  that are obtained by regular subdivision of the reference simplex  $\hat{K}$ . We define for any  $q \in \mathbb{N}_0$ ,

$$N_q := \dim(\mathcal{S}^{q,0}(\hat{K},\hat{\mathcal{I}}_0)) = \binom{q+d}{d},$$

and, for d = 1, 2, ... and q = 0, 1, ...,

$$\tilde{N}_q := \dim(\mathcal{S}^{q,0}(\hat{K},\hat{T}_1) \cap \mathcal{S}^{q,0}(\hat{K},\hat{T}_0)^{\perp}) = (2^d - 1) \begin{pmatrix} q+d \\ d \end{pmatrix}.$$

Denote by  $\{\hat{\varphi}_n\}_{n=1}^{N_q}$  an  $L^2(\hat{K})$  orthonormal basis of

$$\hat{W}_0 := \mathcal{S}^{q,0}(\hat{K}, \hat{\mathcal{T}}_0) = \mathcal{P}_q(\hat{K})$$

and by  $\{\hat{\psi}_n\}_{n=1}^{\hat{N}_q}$  an  $L^2(\hat{K})$  orthonormal basis of

$$\hat{W}_1 := \mathcal{S}^{q,0}(\hat{K}, \hat{\mathcal{T}}_1) \cap \mathcal{S}^{q,0}(\hat{K}, \hat{\mathcal{T}}_0)^{\perp}.$$
(6.6)

For l = 0 we define the basis  $\Psi_0$  by

$$\Psi_0 := \{ (\psi_0)_{j,n} | \forall (K_0)_j \in \mathcal{T}_0 : (\psi_0)_{j,n}|_{(K_0)_j} \circ (F_0)_j = \hat{\varphi}_n, ; \hat{\varphi}_k \in \hat{W}_0 \}$$
(6.7)

and, for every  $l \ge 1$ , we define  $\Psi_l$  by

$$\Psi_l := \{ (\psi_l)_{j,n} : j = 1, \dots, \#(\mathcal{T}_{l-1}), \ n = 1, \dots, N_q \},$$
(6.8)

i.e. by the set of affine images of the (mother-wavelets)  $\hat{\psi}_n$  under  $(F_{l-1})_j$ :

$$(\psi_l)_{j,n} \circ (F_{l-1})_j = \hat{\psi}_n, \quad l \ge 1, \quad j = 1, \dots, \#(\mathcal{T}_{l-1}), \quad n = 1, \dots, \tilde{N}_q$$

By construction,  $(\psi_l)_{j,n} = \hat{\psi}_k \circ ((F_{l-1})_j)^{-1}$  forms an  $L^2(D)$  orthogonal system.

**Proposition 6.1** Assume that the elements  $(\psi_l)_{j,n}$  of the sets  $\Psi_l$  defined in Eqs. (6.7) and (6.8) are  $L^2(D)$  normalized, i.e. that

$$((\psi_l)_{j,n}, (\psi_{l'})_{j',n'})_{L^2(D)} = \delta_{l,l'} \delta_{j,j'} \delta_{n,n'}, \quad \forall l, \ l' \in \mathbb{N}_0,$$
  
$$j = 1, \dots, \#(\mathcal{T}_l), \ j' = 1, \dots, \#(\mathcal{T}_{l'}).$$

Then

$$L^{2}(D) = \bigoplus_{l=0}^{\infty} R_{l}, \quad where \ R_{l} := \operatorname{span}\{\Psi_{l}\}, \quad l \ge 0.$$
(6.9)

*Proof* Since the  $(\psi_l)_{j,n}$  are  $L^2(D)$  orthonormal by construction, the algebraic sums  $\Psi_0 + \Psi_1 + \cdots$  of subspaces are direct. Since, for every  $L \in \mathbb{N}_0$  and every  $q \in \mathbb{N}_0$ 

$$\mathcal{S}^{q,0}(D,\mathcal{T}_L) = \bigoplus_{l=0}^L \Psi_l \supseteq \mathcal{S}^{0,0}(D,\mathcal{T}_L)$$
(6.10)

and since the space of simple functions on the partition  $\mathcal{T}_L$  coincides with  $\mathcal{S}^{0,0}(D, \mathcal{T}_L)$ , the sequence of subspaces defined in Eq. (6.10) is dense in  $L^2(D)$  as  $L \to \infty$ , which proves Eq. (6.9).

Every stochastic diffusion coefficient  $a(\omega, x) \in L^2(\Omega; L^2(D)) = L^2(\Omega, \mathcal{A}, \mathbb{P}; L^2(D))$ admits, by Eq. (6.9), a multi-wavelet expansion

$$a(\omega, x) = \sum_{l=0}^{\infty} \sum_{j=1}^{\bar{N}_l} \sum_{n=1}^{\bar{N}_q} (a_l)_{j,n}(\omega)(\psi_l)_{j,n}(x),$$
(6.11)

where the "coefficients"  $(a_l)_{j,n}(\omega) \in L^2(\Omega, \mathcal{A}, \mathbb{P}; \mathbb{R})$  are random variables defined by

$$(a_l)_{j,n}(\omega) = \int_D a(\omega, x)(\psi_l)_{j,n}(x) \, dx = (a(\omega, \cdot), (\psi_l)_{j,n})_{L^2(D)}.$$
 (6.12)

The convergence in Eq. (6.11) is, as in the case of the Karhunen–Loève expansion, in  $L^2(\Omega, L^2(D))$ . However, unlike in the case of a Karhunen–Loève expansion, in certain cases the Finite Element discretization of Eq. (4.2) on mesh  $\mathcal{T}_L$  coincides *exactly* with the discretization of a diffusion problem where the wavelet coefficient expansion, Eq. (6.11), is truncated at level *L*.

**Proposition 6.2** Assume that the stochastic coefficient  $a(\omega, x)$  in Eq. (3.1) is given in the form of Eq. (6.11). Denote for  $1 \le L < \infty$  by  $a_L(\omega, x)$  the partial sum

$$a_L(\omega, \cdot) = \sum_{l=0}^{L} \sum_{j=1}^{\tilde{N}_l} \sum_{n=1}^{\tilde{N}_q} (a_l)_{j,n}(\omega)(\psi_l)_{j,n}$$
(6.13)

and define the corresponding bilinear form  $B_L(\cdot, \cdot)$  by

$$B_L(v,w) = \mathbb{E}\left[\int_D a_L(\omega,x)\nabla_x v \cdot \nabla_x w \, dx\right], \quad v,w \in L^2(\Omega;V).$$
(6.14)

Then, under the assumption

$$q \ge 2p - 2,\tag{6.15}$$



Fig. 2  $\tilde{N}_q = 3$  Mother-multi-wavelets in Eq. (6.6) for q = 0 and d = 2

the bilinear forms  $B(\cdot, \cdot)$  in Eq. (3.6) and  $B_L(\cdot, \cdot)$  in Eq. (6.14) coincide on the FE spaces  $S^{p,1}(D, T_L)$ :

$$\forall v_L, w_L \in L^2(\Omega; \mathcal{S}^{p,1}(D, \mathcal{T}_L)) : B(v_L, w_L) = B_L(v_L, w_L).$$
(6.16)

*Proof* The proof follows from the definition of  $B(\cdot, \cdot)$  and of  $B_L(\cdot, \cdot)$ , upon noting that by Eq. (6.5) for every  $v_L, w_L \in S^{p,1}(D, \mathcal{T}_L)$  it holds that  $\nabla v_L \cdot \nabla w_L \in S^{2p-2,0}(D, \mathcal{T}_L)$ . The orthogonal sum property of the decomposition in Eq. (6.9) then implies with Eq. (6.15) the assertion.

*Remark 6.3* The identity, Eq. (6.16), has the important implication that in the MLMC-FE method, in *one Finite Element simulation at mesh level l* the bilinear form  $B(\cdot, \cdot)$  can be evaluated on the *exact* stochastic diffusion coefficient  $a(\omega, x)$  in Eq. (6.11) with  $\mathcal{O}(N_l)$  work. This is easily verified from Eq. (6.13) together with the identity in Eq. (6.16).

*Remark 6.4* From Eq. (6.15) and Remark 5.9 we see that for linear scaling MLMC-FE methods for the most important spatial dimensions d = 2, 3, piecewise constant (i.e. q = 0 for p = 1) and piecewise quadratic (i.e. q = 2 for p = 2) discontinuous multiwavelets will have to be used in the wavelet representation, Eq. (6.11), of the stochastic diffusion coefficient. For q = 0 in spatial dimension d = 2, the  $\tilde{N}_q = 3$ generating mother-wavelets  $\hat{\psi}_n$  are shown in Fig. 2.

6.2 Numerical example on D = [0, 1]

In our implementation the mesh  $\mathcal{T}_l$  at level l is the family of intervals of the form  $[(i-1)2^{-l}, i2^{-l}]$  for  $i = 1, ..., 2^l$ , the mesh width is then given by  $h_l = 2^{-l}h_0 = 2^{-l}$ , with  $2^l$  elements per level. This results in a 1-shape regular mesh and the family  $\{\mathcal{T}_l\}_{l=1}^\infty$  is nested. Here we employ Dirichlet boundary conditions, i.e.  $S_{\Gamma_D}^{1,0}(D, \mathcal{T}_0) = S^{1,0}(D, \mathcal{T}_0) \cap H_0^1(D) = \{0\}$ , which implies no degrees of freedom on the boundary.

The hat basis  $(b_l)_i$  at each level l is defined, for  $i = 1, ..., 2^l - 1$ , as:

$$(b_l)_i(x) = 2^l \begin{cases} x - (i-1)h_l & \text{for } x \in [(i-1)h_l, ih_l], \\ (i+1)h_l - x & \text{for } x \in [ih_l, (i+1)h_l], \\ 0 & \text{otherwise.} \end{cases}$$
(6.17)

We consider the following example adapted from [6]

*Example 6.5* Let D = [0, 1],  $\mathbb{E}_a(x) = 5 + x$ ,  $q_a(x, x') = \frac{\min\{x, x'\}+1}{2} \in H^1(D) \otimes H^1(D)$ . The corresponding eigenpairs in the Karhunen–Loève expansion are given by  $\tilde{\lambda}_m = \frac{8}{\pi^2(2m-1)^2}$ ,  $\tilde{\phi}_m(x) = \sin((x+1)/\sqrt{2\tilde{\lambda}_m})$ , for  $m \ge 1$ . The eigenvalues feature algebraic decay with rate 2. The data f, on the right hand side of Eq. (3.1), is set equal to 1.

The diffusion coefficient *a* expressed in the Karhunen–Loève expansion (see Eq. (6.3)) was truncated after the first term. This is then defined as the exact coefficient, avoiding an additional error for the truncation of the Karhunen–Loève expansion. So with an [-1, 1]-uniformly distributed random variable  $Y_1$  we define

$$a_1(\omega, x) := 5 + x + \frac{2\sqrt{2}}{\pi} \cdot Y_1(\omega) \cdot \sin\left(\frac{\pi(x+1)}{4}\right).$$

To establish the error bounds, proven in the previous chapters, in simulations we calculate the exact solution of Eq. (3.1). Therefore, we integrate Eq. (3.1), given the stochastic diffusion coefficient  $a_1$  and the right hand side f = 1, to obtain for the first moment:

$$\mathbb{E}[u(\omega, x)] = \sum_{i=0}^{\infty} \frac{2\sqrt{2}}{\pi(2i+1)} \int_{0}^{x} \frac{c-y}{5+y} \left(\frac{\sin\left(\frac{\pi(y+1)}{4}\right)}{5+y}\right)^{2i} dy,$$

The constant *c* is the solution of the above expression set to zero when integrating over the whole domain D = [0, 1]. The integral was calculated with Mathematica,<sup>2</sup> terminating the sum after i = 5, this leads to  $c \approx 0.4850$ . The integration in each term in the sum is tedious. For the simulations we terminate the series after i = 5. The  $L^2$ -norm between the expansion up to i = 4 and to  $i \ge 5$  is of order  $O(10^{-10})$ . Up to level L = 10, where  $h_L \approx 10^{-3}$  we can neglect the remainder of the series. This error is insignificant given the accuracy of the approximation for simulations up to level L = 10 for point estimates and for the  $L^2$ -norm on the domain D = [0, 1].

The error estimates are calculated in the first order Sobolev semi-norm accordingly, given in Eq. (3.5). The *m*th order Sobolev semi-norm, for  $m \in \mathbb{N}$ , for sufficiently smooth  $u : D \to \mathbb{R}$  is defined as

$$|u|_{H^m(D)}^2 := \sum_{\alpha \in \mathbb{N}^d, |\alpha| \le m} \int_D |D^\alpha u|^2 \, dx.$$

<sup>&</sup>lt;sup>2</sup> Wolfram Research, Inc., Mathematica, Version 7.0; Champaign, IL (2008).

For  $u_l \in V_l = S_{\Gamma_D}^{1,1}(D, \mathcal{T}_l)$  we have

$$|u_l|_{H^1(D)}^2 = \int_D \left(\sum_{i=1}^{2^l-1} (u_l)_i \nabla(b_l)_i(x)\right) \left(\sum_{i=1}^{2^l-1} (u_l)_i \nabla(b_l)_i(x)\right) dx.$$

If we denote by  $S_l$  the stiffness matrix of the Laplace operator with respect to the nodal hat basis  $b_l$  at level l we may write

$$|u_l|_{H^1(D)} = (u_l^\top S_l u_l)^{1/2} \tag{6.18}$$

The simulation was carried out on a Computer with a 2 GHz processor with one GB RAM using MATLAB.<sup>3</sup> As a solver we used the backslash operator, mldivide, in MATLAB.

#### 6.2.1 *MLMC-FE* method for the approximation of $\mathbb{E}[u]$

Our aim is to verify the theoretical approximation error for the MLMC-FE method  $||\mathbb{E}[u] - E^{L}[u]||_{L^{2}(\Omega;V)}$ , given in Theorem 4.5. Therefore, we consider the nested family  $\{\mathcal{T}_{l}\}_{l=1}^{L}$  of meshes and the FE spaces  $V_{l} = S^{1,1}(D, T_{l})$  with basis functions  $\{(b_{l})_{i}\}_{i=1}^{2^{l}-1}$ , defined in Eq. (6.17), on each level  $l = 1, \ldots, L$ . Each level is constructed by adding the mid points between two vertices to the mesh of the previous level. Thus, we get  $2^{(l-1)}$  additional linear independent basis functions passing from  $V_{l-1}$  to  $V_{l}$ . To construct the single scale basis  $\{(b_{l})_{i}\}_{i=1}^{2^{l}-1}$ , we transform each basis function of level l - 1 into the basis function of level l plus  $2^{(l-1)}$  additional basis functions. This allows us to calculate  $E^{L}[u]$ , since we need to subtract the solution in  $V_{l-1}$  from the solution in  $V_{l}$  (see Eq. (4.9)). For each sample of the stochastic coefficient on each level we assemble the stiffness matrix and solve the deterministic system of equations, given in Eq. (3.6), to obtain  $u_{l}^{i}$ . With this and the exact solution we get with Eq. (6.18) the desired error.

The rate of convergence of the MLMC-FE approximation, depending on the level L, is displayed in Fig. 3a. The asymptotic convergence rate predicted by Theorem 4.5,  $O(h_L)$ , is visible in the simulation (as indicated by the reference slope). Figure 4a shows the total CPU-time needed to calculate  $E^L[u]$  for different levels L. It reflects the calculated expected behavior of the total work  $Work(L) \leq C_{\epsilon} N_L^2$  in Theorem 4.5 for d = 1. In Fig. 5a is the CPU-time per sublevel l, for l = 1, ..., L, depicted. For sample sizes  $M_l$  as in Theorem 4.5 the CPU-time at each sublevel l is of rate  $O(l^2 2^{-l})$ .

*Remark 6.6* We remark that for the numerical results we calculated  $\|\mathbb{E}[u] - E^{L}[u]\|_{V}$ instead of  $\|\mathbb{E}[u] - E^{L}[u]\|_{L^{2}(\Omega;V)}$ . The order of the convergence rate is obviously identical. If we approximate  $\mathbb{E}\|\mathbb{E}[u] - E^{L}[u]\|_{V}^{2}$  by  $\frac{1}{\eta}\sum_{i=1}^{\eta}\|\mathbb{E}[u] - E^{L}[u]^{i}\|_{V}^{2}$  one calculates with  $\mathbb{P}(\frac{1}{\eta}\sum_{i=1}^{\eta}\|\mathbb{E}[u] - E^{L}[u]^{i}\|_{V}^{2} > \epsilon) \leq C$  the  $\eta$  for a given confidence

<sup>&</sup>lt;sup>3</sup> MATLAB, version 7.9.0.529 (R2009b); Natick, MA: The MathWorks Inc., 2009.



**Fig. 3** Rate of convergence of the MLMC-FE method with respect to the  $H^1$ -semi-norm for the approximation of  $\mathbb{E}(u)$  in (**a**) and  $\mathcal{M}^2(u)$  in (**b**) in dimension d = 1 against the level



**Fig. 4** Total CPU time for the MLMC–FE approximation of  $E^{L}(u)$  in (**a**) and  $\mathcal{M}^{2}(u)$  in (**b**) in 1*d* against the level

level C, here  $\epsilon$  is an upper bound for the total error, i.e. the combined statistical and discretization error.

# 6.2.2 MLMC-FE method for the approximation of $\mathcal{M}^2[u]$

The calculation of the second moment  $\mathcal{M}^2 u$  is performed in three steps. First, compute the Finite Element solution in a standard nodal hat basis for a given level *l*, as described above, to compute  $u_l^i$ . In a second step, we transform the result into a hierarchic B-spline linear wavelet basis. Finally, in a third step, we generate the sparse tensor product by implementing Eq. (5.6), the sparse tensor projection. This algorithm is repeated for each level and, according to Eq. (5.8), this leads to the MLMC-FE approximation  $\hat{E}^L((u_L)^2)$  of  $\mathcal{M}^2 u$ .

In Fig. 3b we compare the sparse tensor product solution to the sparse tensor product of the solution  $\hat{E}^{L}((u_{L+4})^2)$ . The error resembles the theoretical results of



**Fig. 5** CPU-time per sublevel for different levels for the MLMC-FE approximation of  $\mathbb{E}(u)$  in (**a**) and  $\mathcal{M}^2(u)$  in (**b**) in dimension d = 1

Theorem 5.7, as the reference slope indicates. The total CPU-time in dependence of the degrees of freedom has quadratic growth as stated in Eq. (5.11), is displayed in Fig. 4b. Figure 5b shows the CPU-time on all sublevels *l*, for l = 1, ..., L for a fixed level *L*. Theoretically this is, for fixed level *L*,  $M_l N_l = O(l 2^{-l})$ , with  $M_l$  as in Theorem 4.5.

# 6.3 Numerical example on $D = [0, 1]^2$

We consider the unit square and define level l = 0 to be the space of the boundary basis functions with four vertices  $P_1 = (0, 0)$ ,  $P_2 = (1, 0)$ ,  $P_3 = (1, 1)$  and  $P_4 = (0, 1)$ , the triangulation of the unit square is given by the triangles  $P_1P_2P_4$  and  $P_2P_3P_4$ . Given the Dirichlet boundary condition the simulation on this level is superfluous. The nested family  $\mathcal{T}_{l+1}$  is constructed by dividing each triangle of level l into four congruent triangles of the same size. The resulting mesh is then  $(2 - \sqrt{2})$ -shape regular. Figure 6a shows the  $\mathcal{T}_2$  mesh. Similar to the example in one space dimension, we apply Dirichlet boundary conditions. We adapt Example 6.5 to  $\mathbb{R}^2$  as follows:

*Example* 6.7 Let  $D = [0, 1]^2$  and choose the sequence  $\{\phi_{mn}\}_{m,n\geq 1}$ , given by  $\phi_{mn}(x, y) = \tilde{\phi}_m(x)\tilde{\phi}_n(y)$  with  $\tilde{\phi}_m$  as in Example 6.5, ordered by the magnitude of the corresponding eigenvalues  $\{\lambda_{mn}\}_{m,n\geq 1}$ . The eigenvalues  $\lambda_m$  are chosen as  $\lambda_m = (\tilde{\lambda}_m)^{\theta}$  with  $\theta = 2.5$ , such that the algebraic decay of  $\{\lambda\}_{m\geq 1}$  is of rate 5/2.

The simulation in dimension d = 2 was carried out on a cluster compute server with AMD Opteron Processors, between 2.4 and 2.8 GHz per core. We used here, as in the case d = 1, the backslash operator to solve each linear system.



**Fig. 6** Grid for level 2 (d = 2) in (**a**) and degrees of freedom versus CPU time for the MLMC-FE approximation of  $\mathcal{M}^2(u)$  in 2d (**b**)

#### 6.3.1 MLMC-FE method for the approximation of $\mathbb{E}[u]$

For d = 2 we did not calculate the exact solution  $\mathbb{E}[u_L]$  as before. In this case the reference solution is either the solution of a Monte Carlo simulation with high sample count (10,000 samples) or the solution of the MLMC-FE simulation on level L + 1. Further, we did not integrate the entries of the stiffness matrix, B given in Eq. (3.6), exactly. Here we use a seven point Gaussian quadrature rule of order 6. Figure 7a shows the error of the MLMC-FE approximation for the mean field in dependence of the level. The theoretical results from Theorem 4.5 are resembled. For the total computational costs we calculated in Theorem 4.5, for d = 2, Work  $(L) = O(N_L (\log N_L)^{3+\epsilon})$ . This is also apparent in Fig. 8a. We deduce that the MLMC-FE method has log-linear computational time, whereas the convergence is the same as in the Monte Carlo method. The results can be compared to those in Fig. 4a for d = 1, where the CPU-time was quadratic. The work load on each sublevel l, for  $l = 1, \ldots, L$  can easily be computed as  $O(l^2)$ , matching the results of the simulation in Fig. 9a.

#### 6.3.2 MLMC-FE method for the second moment

For the calculation of the error of the MLMC-FE method for  $\mathcal{M}^2[u]$  we proceed as in the one-dimensional case. Results in Fig. 7b reflect the theoretical error for the MLMC-FE approximation of rate  $O(h_L(\log h_L)^{3/2})$  as stated in Theorem 5.7 for k = 2and s = 1. Equally the simulation results on the total CPU-time pictured in Fig. 8b for the asymptotic bound on the overall work, Eq. (5.11) ( $\widehat{W}(L) = O(N_L(\log N_L))$ ), slight differences in the rate of convergence are due to the non-optimal complexity of the backslash operator for large systems. This points to the use of a Multigrid method to achieve optimal results for large *L*. For the CPU-time on the sublevels *l*, for  $l = 1, \ldots, L$ , we have a linear growth with increasing sublevel. This can be easily calculated with  $M_l$  as in Eq. (5.10) and  $N_l = 2^{2l}$ . The results shown in Fig. 9b are



**Fig. 7** Rate of convergence of the MLMC-FE method with respect to the  $H^1$ -semi-norm for the approximation of  $\mathbb{E}(u)$  in (**a**) and  $\mathcal{M}^2(u)$  in (**b**) in dimension d = 2 against the level



**Fig. 8** Total CPU time for the MLMC-FE approximation of  $E^{L}(u)$  in (**a**) and  $\mathcal{M}^{2}(u)$  in (**b**) in 2*d* against the level

influenced the most by the generation of the sparse tensor product (see Fig. 6b), such that the linear scaling is not fully visible here.

*Remark 6.8* The serial Monte Carlo and therefore the MLMC-FE simulations can easily be implemented for parallel computing. No communication between processes is needed during execution if available memory allows for the handling of one sample on one processor. This means load balancing can easily be achieved without the need for communication between the processors during execution. However, the random number streams for each processor should exhibit low correlation between streams. The results are gathered at the end of the computation. In the case of a single-level MC-FE method each result can be added independently to the result of any other processor and data loss only leads to a reduction in the convergence speed. In the case of a MLMC-FE method the correct order of summation of the final result on each level has to be respected. This means that the MLMC-FE simulation is much more sensitive



**Fig. 9** CPU-time per sublevel for different levels for the MLMC-FE approximation of  $\mathbb{E}(u)$  in (**a**) and  $\mathcal{M}^2(u)$  in (**b**) in dimension d = 2

to data loss then is the MC-FE simulation. In our example the sample size of the finest level was normalized to one. In dimension d = 1 for the calculation of the mean field and the second moment we have decreasing load with increasing mesh refinements (see Fig. 5). If the calculation on the finest sublevel (normalized to one sample) can be performed on one processor, we can balance the work load for the other sublevels, with higher work load due to higher sample sizes, by splitting the sampling streams to more than one processor. In the case of spatial dimension  $d \ge 2$ , however, the complexity of sampling on the finest mesh usually exceeds the capacity of a single processor. In this case, load balancing and linear scaling can only be achieved by domain decomposition, or, depending on the number of processors available, both, domain decomposition and sample splitting (see [26]).

For all the simulations we truncated the sum in the Karhunen–Loève expansion after the first term. This truncation could be coupled to the degrees of freedom of the spatial approximation as well, or it could be fixed to some higher term. This leads to a more complex calculation of the exact solution and the stiffness matrix, but also to an error reduction in the approximation of the exact moments of the solution. An algorithm to generate correlated Gaussian random fields is given in [23].

#### 7 Conclusions

Our error and complexity analysis reveals that for low order Finite Element discretizations in the physical domain *D*, the proposed MLMC-FE method achieves an approximation of the mean field of the random solution and its *k*th moments with *efficiency* (*i.e. error versus computational work*) which is comparable to one solve of a linear complexity Finite Element method for a deterministic elliptic problem of the same type.

Our error and complexity analysis also shows that *preservation of increased conver*gence rates of higher order Finite Element methods for the approximation of stochastic solutions with higher spatial regularity entails corresponding increase of the MC samples at each mesh level. This implies a loss of the overall log-linear complexity of the MLMC-FE scheme. For problems with random solutions that exhibit high spacial smoothness as well as high summability, higher convergence rates of the overall discretization scheme will require apart from high order Finite Element methods in the physical domain also improved discretization strategies in the stochastic domain such as spectral, polynomial chaos based discretizations (see, e.g. [1,2,6,7,11,12,29,30]).

Therefore, the MLMC-FE method proposed here is competitive for stochastic PDE problems whose solutions have low smoothness in physical space, and moderate summability in  $\omega \in \Omega$  as, e.g. finite second moments. This is typically the case in Gaussian models of porous media where realizations of *a* are, roughly speaking, Hölder continuous with exponent at most 1/2.

In closing, we emphasize that the presently proposed MLMC-FE method does not require stationarity or Gaussianity of the stochastic diffusion coefficient a in any way. For stationary, Gaussian random inputs, linear scaling simulation methods can be built on tensorized Fast Fourier Transform algorithms (see, e.g. [14] and the references therein). Both methods proposed here, the Karhunen–Loève based and the wavelet based parametrization of  $a(\omega, x)$ , allow for non-stationary and irregular random inputs.

The representations in Eqs. (6.11) and (6.13) can, due to the  $L^2(D)$  orthogonality in Eq. (6.12) of the (multi) wavelets be utilized *directly* in scenario generation based on a stream of "coefficient realizations" of *a*, possibly in digital form with uniform pixel resolution  $\geq L$ . In this case, Eq. (6.16) implies that a "forward" MLMC-FE simulation on mesh  $T_L$  can account for all available data on *a exactly*.

Finally, we indicate that the MLMC approach is rather general: for an application to hyperbolic conservation laws, see [25,26].

#### References

- 1. Babuška I., Nobile F., Tempone R.: A stochastic collocation method for elliptic partial differential equations with random input data. SIAM J. Numer. Anal. 45, 1005–1034 (2007, electronic)
- Babuška, I., Tempone, R., Zouraris, G.E.: Galerkin Finite Element approximations of stochastic elliptic partial differential equations. SIAM J. Numer. Anal., 42, 800–825 (2004, electronic)
- Barth, A.: A Finite Element Method for martingale-driven stochastic partial differential equations. Commun. Stoch. Anal. 4, 355–375 (2010)
- Barth, A., Lang, A.: Almost sure convergence of a Galerkin–Milstein approximation for stochastic partial differential equations. Tech. Report 2011–15. Seminar for Applied Mathematics, ETH Zurich, March 2009 (in review)
- Barth, A., Lang, A.: Simulation of stochastic partial differential equations using Finite Element methods. Stochastics (2010, in press)
- Bieri, M., Andreev, R., Schwab, C.: Sparse tensor discretization of elliptic SPDEs. SIAM J. Sci. Comput. 31, 4281–4304 (2009/2010)
- Bieri, M., Schwab, C.: Sparse high order FEM for elliptic sPDEs. Comput. Methods Appl. Mech. Eng. 198, 1149–1170 (2009)
- 8. Braess, D.: Finite Elemente, 3rd edn. Springer, Berlin (2002)
- Brenner, S.C., Scott, L.R.: The Mathematical Theory of Finite Element Methods, 2nd edn. Springer, Berlin (2002)
- Cohen, A.: Numerical analysis of wavelet methods. In: Studies in Mathematics and its Applications. North-Holland, Amsterdam (2003)

- 11. Cohen, A., DeVore, R., Schwab, C.: Convergence rates of best *n*-term approximations for a class of elliptic spdes. Found. Comput. Math. **10**, 615–646 (2010)
- Cohen, A., DeVore, R., Schwab, C.: Analytic regularity and polynomial approximation of parametric and stochastic elliptic PDEs. J. Anal. Appl. 9, 11–47 (2011)
- Da Prato, G., Zabczyk, J.: Stochastic equations in infinite dimensions. Encyclopedia of Mathematics and its Applications, vol. 44. Cambridge University Press, Cambridge (1992)
- Dietrich, C.R., Newsam, G.N.: Fast and exact simulation of stationary Gaussian processes through circulant embedding of the covariance matrix. SIAM J. Sci. Comput. 18, 1088–1107 (1997)
- Geissert, M., Kovács, M., Larsson, S.: Rate of weak convergence of the Finite Element Method for the stochastic heat equation with additive noise. BIT Numer. Math. 49, 343–356 (2009)
- Gilbarg D., Trudinger N.S.: Elliptic partial differential equations of second order. In: Classics in Mathematics. Springer, Berlin (2001, reprint of the 1998 edition)
- Giles, M.: Improved multilevel Monte Carlo convergence using the Milstein scheme. Preprint NA-06/22. Oxford University Computing Laboratory, Parks Road (2006)
- 18. Giles, M.B.: Multilevel Monte Carlo path simulation. Oper. Res. 56, 607-617 (2008)
- Griebel, M., Oswald, P.: On additive Schwarz preconditioners for sparse grid discretizations. Numer. Math. 66, 449–463 (1994)
- Grisvard, P.: Elliptic problems in nonsmooth domains. Monographs and Studies in Mathematics, vol. 24. Pitman (Advanced Publishing Program), Boston (1985)
- Heinrich, S.: Multilevel Monte Carlo Methods. In: Large-Scale Scientific Computing, Third International Conference, LSSC 2001, Sozopol, Bulgaria, June 6–10, 2001 (Revised Papers, S. Margenov, J. Wasniewski, and P. Y. Yalamov, eds., vol. 2179 of Lecture Notes in Computer Science, Springer, 2001, pp. 58–67)
- Kovács, M., Larsson, S., Saedpanah, F.: Finite Element approximation of the linear stochastic wave equation with additive noise. SIAM J. Numer. Anal. 48, 408–427 (2010)
- 23. Lang A., Potthoff J.: Fast simulation of Gaussian random fields (2009, in review)
- Lions, J.-L., Magenes E.: Non-homogeneous boundary value problems and applications, vol. I. Springer-Verlag, New York (1972). (Translated from the French by P. Kenneth, Die Grundlehren der mathematischen Wissenschaften, Band 181)
- Mishra S., Schwab C.: Sparse tensor Multi-Level Monte Carlo Finite Volume Methods for hyperbolic conservation laws with random initial data. Tech. Report 2010-24. Seminar for Applied Mathematics, ETH Zurich, September 2010 (in review)
- Mishra S., Schwab C., Šukys J.: Multi-Level Monte Carlo Finite Volume Mmethods for nonlinear systems of conservation laws in multi-dimensions with random initial data. Tech. Report 2011-02. Seminar for Applied Mathematics, ETH Zurich, January 2011 (in review)
- Naff, R.L., Haley, D.F., Sudicky, E.: High-resolution Monte Carlo simulation of flow and conservative transport in heterogeneous porous media 1. Methodology and flow results. Water Resour. Res. 34, 663–677 (1998)
- Naff, R.L., Haley, D.F., Sudicky, E.: High-resolution Monte Carlo simulation of flow and conservative transport in heterogeneous porous media 2. Transport results. Water Resour. Res. 34, 679–697 (1998)
- Nobile, F., Tempone, R., Webster, C.G.: An anisotropic sparse grid stochastic collocation method for partial differential equations with random input data. SIAM J. Numer. Anal. 46, 2411–2442 (2008)
- Nobile, F., Tempone, R., Webster, C.G.: A sparse grid stochastic collocation method for partial differential equations with random input data. SIAM J. Numer. Anal. 46, 2309–2345 (2008)
- Schwab, C., Todor, R.A.: Sparse Finite Elements for elliptic problems with stochastic loading. Numer. Math. 95, 707–734 (2003)
- 32. Schwab, C., Todor, R.A.: Sparse Finite Elements for stochastic elliptic problems—higher order moments. Computing **71**, 43–63 (2003)
- Schwab, C., Todor, R.A.: Karhunen–Loève approximation of random fields by generalized fast multipole methods. J. Comput. Phys. 217, 100–122 (2006)
- von Petersdorff, T., Schwab, C.: Numerical solution of parabolic equations in high dimensions. M2AN Math. Model. Numer. Anal. 38, 93–127 (2004)