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## Multi-level quasi-Monte Carlo finite element methods for a class of elliptic partial differential equations with random coefficients

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**Abstract** Quasi-Monte Carlo (QMC) methods are applied to multi-level Finite Element (FE) discretizations of elliptic partial differential equations (PDEs) with a random coefficient. The representation of the random coefficient is assumed to require a countably infinite number of terms.

The multi-level FE discretizations are combined with families of QMC methods (specifically, randomly shifted lattice rules) to estimate expected values of linear functionals of the solution, as in [17, 18, 23] in the single-level setting. Here, the expected value is considered as an infinite-dimensional integral in the parameter space corresponding to the randomness induced by the random coefficient. In this paper we study the same model as in [23]. The error analysis of [23] is generalized to a multi-level scheme, with the number of QMC points depending on the discretization level, and with a level-dependent dimension truncation strategy. In some scenarios, it is shown that the overall error of the expected value of the functionals of the solution (i.e., the root-mean-square error averaged over all shifts) is of order  $\mathcal{O}(h^2)$ , where  $h$  is the finest FE mesh width, or  $\mathcal{O}(N^{-1+\delta})$  for arbitrary  $\delta > 0$ , where  $N$  denotes the maximal number of QMC sampling points in the parameter space. For these scenarios, the total work for all PDE solves in the multi-level QMC-FE method is shown to be essentially of the order of *one single PDE solve at the finest FE discretization level*, for spatial dimension  $d \geq 2$  with linear elements.

The analysis exploits regularity of the parametric solution with respect to both the physical variables (the variables in the physical domain) and the parametric vari-

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ables (the parameters corresponding to randomness). As in [23], families of QMC rules with ‘‘POD weights’’ (‘‘product and order dependent weights’’) which quantify the relative importance of subsets of the variables are found to be natural for proving convergence rates of QMC errors that are independent of the number of parametric variables. Our POD weights for the multi-level QMC-FE algorithm are different from those for the single-level algorithm in [23]. Conditions on the data of the problem to achieve a certain rate of convergence coincide with the sufficient conditions obtained in [6] to achieve the same convergence rates for best  $N$ -term approximations of solutions for the parametric PDE model.

**Keywords** Multi-level · Quasi-Monte Carlo methods · Infinite dimensional integration · Elliptic partial differential equations with random coefficients · Karhunen-Loève expansion · Finite element methods

**Mathematics Subject Classification (2000)** 65D30 · 65D32 · 65N30

## 1 Introduction

This paper is a sequel to our work [23], where we analyzed theoretically the application of quasi-Monte Carlo (QMC) methods combined with finite element (FE) methods for a scalar, second order elliptic partial differential equation (PDE) with random diffusion. The diffusion is assumed to be given as an infinite series with random coefficients. As in [23], we consider the model parametric elliptic Dirichlet problem

$$-\nabla \cdot (a(\mathbf{x}, \mathbf{y}) \nabla u(\mathbf{x}, \mathbf{y})) = f(\mathbf{x}) \quad \text{in } D \subset \mathbb{R}^d, \quad u(\mathbf{x}, \mathbf{y}) = 0 \quad \text{on } \partial D, \quad (1)$$

for  $D \subset \mathbb{R}^d$  a bounded domain with a Lipschitz boundary  $\partial D$ . In (1), the gradients are understood to be with respect to the physical variable  $\mathbf{x}$  which belongs to  $D$ , and the parameter vector  $\mathbf{y} = (y_j)_{j \geq 1}$  consists of a countable number of parameters  $y_j$  which we assume, as in [23], to be i.i.d. uniformly distributed, with

$$\mathbf{y} \in \left(-\frac{1}{2}, \frac{1}{2}\right)^{\mathbb{N}} =: U.$$

The parameter  $\mathbf{y}$  is thus distributed on  $U$  with the uniform probability measure  $\mu(d\mathbf{y}) = \otimes_{j \geq 1} dy_j = d\mathbf{y}$ . The parametric diffusion coefficient  $a(\mathbf{x}, \mathbf{y})$  in (1) is assumed to depend linearly on the parameters  $y_j$  as follows:

$$a(\mathbf{x}, \mathbf{y}) = \bar{a}(\mathbf{x}) + \sum_{j \geq 1} y_j \psi_j(\mathbf{x}), \quad \mathbf{x} \in D, \quad \mathbf{y} \in U. \quad (2)$$

The  $\psi_j$  can either be Karhunen-Loève eigenfunctions (see, e.g. [31]), or other suitable function systems in  $L^2(D)$ . As in [23] we impose a number of assumptions on  $\bar{a}$  and  $\psi_j$  as well as on the domain  $D$ :

- (A1) We have  $\bar{a} \in L^\infty(D)$  and  $\sum_{j \geq 1} \|\psi_j\|_{L^\infty(D)} < \infty$ .
- (A2) There exist  $a_{\max}$  and  $a_{\min}$  such that  $0 < a_{\min} \leq a(\mathbf{x}, \mathbf{y}) \leq a_{\max}$  for all  $\mathbf{x} \in D$  and  $\mathbf{y} \in U$ .
- (A3) There exists  $p \in (0, 1)$  such that  $\sum_{j \geq 1} \|\psi_j\|_{L^\infty(D)}^p < \infty$ .

- (A4) With the norm  $\|v\|_{W^{1,\infty}(D)} := \max\{\|v\|_{L^\infty(D)}, \|\nabla v\|_{L^\infty(D)}\}$ , we have  $\bar{a} \in W^{1,\infty}(D)$  and  $\sum_{j \geq 1} \|\psi_j\|_{W^{1,\infty}(D)} < \infty$ .
- (A5) The sequence  $\psi_j$  is ordered so that  $\|\psi_1\|_{L^\infty(D)} \geq \|\psi_2\|_{L^\infty(D)} \geq \dots$ .
- (A6) The domain  $D$  is a convex and bounded polyhedron with plane faces.

We now briefly comment on each assumption. Assumption (A1) ensures that the coefficient  $a(\mathbf{x}, \mathbf{y})$  is well-defined for all parameters  $\mathbf{y} \in U$ . Assumption (A2) yields the strong ellipticity needed for the standard FE analysis. Assumption (A3) is stronger than Assumption (A1). This assumption implies decay of the fluctuation coefficients  $\psi_j$ , with faster decay for smaller  $p$ . The value of  $p$  determined the convergence rate in the previous paper [23]. Assumption (A4) guarantees that the FE solutions converge. Assumption (A5) allows the truncation of the infinite sum in (2) to, say,  $s$  terms. This assumption is not needed in this paper when the functions  $\psi_j$  satisfy an orthogonality property in relation to the FE spaces, see §3.3 below. Finally, Assumption (A6) only simplifies the FE analysis and can be substantially relaxed.

Our aim in this paper is to extend the QMC-FE algorithm of [23] for the efficient computation of expected values of continuous linear functionals of the solution of (1) to a *multi-level* setting so that the overall computational cost is substantially reduced. Suppose the linear functional is  $G(\cdot) : H_0^1(D) \mapsto \mathbb{R}$ . We are interested in approximating the integral

$$\begin{aligned} I(G(u)) &:= \int_U G(u(\cdot, \mathbf{y})) \, d\mathbf{y} \\ &:= \lim_{s \rightarrow \infty} \int_{(-\frac{1}{2}, \frac{1}{2})^s} G(u(\cdot, (y_1, \dots, y_s, 0, 0, \dots))) \, dy_1 \cdots dy_s. \end{aligned} \quad (3)$$

The (single level) strategy in [23] was to (i) truncate the infinite sum in the expansion of the coefficient to  $s$  terms, (ii) approximate the solution of the truncated PDE problem using a FE method with mesh width  $h$ , and (iii) approximate the integral using a QMC method (an equal-weight quadrature rule) with  $N$  points in  $s$  dimensions. The QMC-FE algorithm can therefore be expressed as

$$Q_{s,N}(G(u_h^s)) := \frac{1}{N} \sum_{i=1}^N G(u_h^s(\cdot, \mathbf{y}^{(i)})),$$

where  $u_h^s$  denotes the FE solution of the truncated PDE problem, and  $\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(N)}$  are QMC sample points which are judiciously chosen from the  $s$ -dimensional unit cube  $[-\frac{1}{2}, \frac{1}{2}]^s$ . More precisely, the QMC rules considered in [23] are *randomly shifted lattice rules*; more details will be given in the next section. It was established in [23] that the root-mean-square of the error  $I(G(u)) - Q_{s,N}(G(u_h^s))$  over all random shifts is a *sum* of three parts: a truncation error, a QMC error, and a FE error. For example, in the particular case where Assumption (A3) holds with  $p = 2/3$  and  $f, G(\cdot) \in L^2(D)$ , it was shown that the three additive parts of the error are of orders  $\mathcal{O}(s^{-1})$ ,  $\mathcal{O}(N^{-1+\delta})$ , and  $\mathcal{O}(h^2) = \mathcal{O}(M_h^{-2/d})$ , respectively, where  $M_h$  is the number of FE nodes and  $d$  is the spatial dimension. Assuming the availability of a linear complexity FE solver in the domain  $D$  (e.g., a multigrid method), the overall cost of the (single level) QMC-FE algorithm is  $\mathcal{O}(sNM_h)$ . There, as in the present paper, we assume that the functions

$\psi_j$  and their (piecewise-constant) gradients are explicitly known, and that integration of any FE basis functions over a single element in the FE mesh is available at unit cost.

The purpose of the present paper is the design and the error-versus-cost analysis of a *multi-level* extension of the single level algorithm developed in [23]. The multi-level algorithm takes the form

$$Q_*^L(G(u)) := \sum_{\ell=0}^L Q_{s_\ell, N_\ell} \left( G(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}}) \right), \quad (4)$$

where  $s_\ell$  is a nondecreasing sequence of truncation dimensions,  $u_{h_\ell}^{s_\ell}$  denotes the FE approximation with mesh width  $h_\ell$  of the PDE problem with parametric input (2) truncated at  $s_\ell$  terms, with the convention  $u_{h_{-1}}^{s_{-1}} \equiv 0$ , and  $Q_{s_\ell, N_\ell}$  denotes the (randomly shifted) QMC quadrature rule with  $N_\ell$  points in  $s_\ell$  dimensions. (For the practical form of the quadrature rule, including randomization, see (20) below.) Assuming again the availability of a linear complexity FE solver in the domain  $D$ , the overall cost of this multi-level QMC-FE algorithm is therefore  $\mathcal{O}(\sum_{\ell=0}^L s_\ell N_\ell M_{h_\ell})$  operations. Again we use randomly shifted lattice rules, and we show that  $s_\ell$ ,  $N_\ell$ , and  $M_{h_\ell}$  enter the root-mean-square of the error  $I(G(u)) - Q_*^L(G(u))$  over all random shifts in a *combined additive and multiplicative manner*. Upon choosing  $s_\ell$  and  $N_\ell$  in relation to  $h_\ell$  appropriately at each level  $\ell$ , we arrive at a dramatically reduced overall cost compared to the single level algorithm.

The general concept of multi-level algorithms was first introduced by Heinrich [19] and reinvented by Giles [14, 15]. Since then the concept has been applied in many areas including high dimensional integration, stochastic differential equations, and several types of PDEs with random coefficients. Most of these works used multi-level Monte Carlo (MC) algorithms, while few papers considered multi-level QMC algorithms. The multi-level QMC-FE algorithm (4) proposed and analyzed here differs in several core aspects from the abstract multi-level QMC framework proposed in [16, 26]. It also differs from the multi-level MC approach which has recently been developed for elliptic problems with random input data of the general form (1) in [2, 3, 5, 30, 35]. The model considered here, as in [23], is infinite-dimensional. Previous treatments of infinite-dimensional quadrature include [16, 24, 26] with QMC methods, [20] with MC methods, and [29] with Smolyak (or sparse-grid) quadrature.

There is an important special case where the functions  $\psi_j$  satisfy an orthogonality property in relation to the FE spaces, see (28) ahead. In this case there is *no dimension truncation error at any level*, that is, with  $s_\ell$  chosen in an appropriate way we have  $u_{h_\ell}^{s_\ell} = u_{h_\ell}$ . Furthermore, due to the special structure of the expansion of the coefficient  $a(\mathbf{x}, \mathbf{y})$ , the overall cost is only  $\mathcal{O}(\sum_{\ell=0}^L N_\ell M_{h_\ell} \log(M_{h_\ell}))$  operations. To have this orthogonality property we need *multiresolution* function systems; examples are given in §3.3. We emphasize that the eigenfunction system of the covariance operator does *not* have this property.

One of the main findings of the present paper is that the error analysis of the multi-level QMC-FE algorithm requires *smoothness of the parametric solution simultaneously with respect to the spatial variable  $\mathbf{x}$  and to the parametric variable  $\mathbf{y}$* .

Another key point is that we require decay of stronger norms of the fluctuation coefficients  $\psi_j$  compared to Assumptions (A3) and (A4):

(A7) For  $p$  as in (A3), there exists  $q \in [p, 1]$  such that  $\sum_{j \geq 1} \|\psi_j\|_{W^{1,\infty}(D)}^q < \infty$ .

For the multi-level QMC-FE algorithm the convergence rate will be determined by the value of  $q$  in (A7) rather than by the value of  $p$  as for the single level algorithm in [23].

As in most modern analyses of QMC integration in high dimensions, we use parameters  $\gamma_u$ , known as *weights*, to describe the relative importance of the subset of the variables with labels in the finite subset  $u \subset \mathbb{N}$ . (These weights are to be distinguished from quadrature weights in, e.g., Gaussian quadrature formulas.) In [23] the weights were chosen to minimize a certain upper bound on the product of the *worst case error* and the norm in the function space, yielding a special form of weights called ‘‘POD weights’’, which stand for ‘‘product and order dependent weights’’:

$$\gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j, \quad (5)$$

where  $|u|$  denotes the cardinality (or the ‘‘order’’) of the set  $u$ . These weights are then determined by the two sequences: by  $\Gamma_0 = 1, \Gamma_1, \Gamma_2, \Gamma_3, \dots$  and by  $\gamma_1, \gamma_2, \gamma_3, \dots$ . The error bound obtained in the present paper is more complicated than the result in [23] due to the multi-level nature of the algorithm, but we follow the same general principle for choosing weights. It turns out that the ‘‘optimal’’ weights (in the sense of minimizing an upper bound on the overall error) for the multi-level QMC-FE algorithm are again POD weights (5), but they are different from the POD weights for the single level algorithm in [23]. In any case, fast CBC construction algorithms for randomly shifted lattice rules are available for POD weights, see [22] for a recent survey, as well as [32, 21, 9, 27, 28, 7, 11].

The outline of this paper is as follows. In §2 we introduce the function spaces used for the analysis and summarize those results from [23] that are needed for this paper. In §3 we prove the main results required for the error analysis and combine them to obtain an error bound for the multi-level QMC-FE algorithm. Finally in §4 we give conclusions.

## 2 Problem Formulation and Summary of Relevant Results

### 2.1 Function Spaces

First we introduce the function spaces from [23] which will be used in what follows. Our variational setting of (1) is based on the Sobolev space  $V = H_0^1(D)$  and its dual space  $V^* = H^{-1}(D)$ , with pivot space  $L^2(D)$ , and with the norm in  $V$  given by

$$\|v\|_V := \|\nabla v\|_{L^2(D)}.$$

We also consider the Hilbert space with additional regularity with respect to  $\mathbf{x}$ ,

$$Z^t := \{v \in V : \Delta v \in H^{-1+t}(D)\}, \quad 0 \leq t \leq 1, \quad (6)$$

with the norm

$$\|v\|_{Z^t} := \left( \|v\|_{L^2(D)}^2 + \|\Delta v\|_{H^{-1+t}(D)}^2 \right)^{1/2}, \quad (7)$$

where, for  $-1 \leq r \leq 2$ , the  $H^r(D)$  norm denotes the homogeneous  $H^r(D)$ -norm which is defined in terms of the  $L^2(D)$  orthonormalized eigenfunctions  $\varphi_\lambda \in V$  and the eigenvalues  $\lambda$  in the corresponding spectrum  $\Sigma$  of the Dirichlet Laplacian in  $D$  by

$$\|v\|_{H^r(D)}^2 := \sum_{\lambda \in \Sigma} \lambda^r |(v, \varphi_\lambda)|^2.$$

Here, and in the following, we denote by  $(\cdot, \cdot)$  the bilinear form corresponding to the  $L^2(D)$  innerproduct, extended by continuity to the duality pairing  $H^r(D) \times H^{-r}(D)$ . Standard elliptic regularity theory (see, e.g. [13]) yields the inclusion  $Z^t \subset H_{\text{loc}}^{1+t}(D)$ , and for convex domains  $D$  and for  $t = 1$  we have  $Z^1 = H^2(D) \cap H_0^1(D)$ . As already seen in §1, we will also make use of the norm

$$\|v\|_{W^{1,\infty}(D)} := \max\{\|v\|_{L^\infty(D)}, \|\nabla v\|_{L^\infty(D)}\}.$$

The integrand in (3) is  $F(\mathbf{y}) := G(u(\cdot, \mathbf{y}))$ . To analyze QMC integration for such integrands, we shall need a function space defined with respect to  $\mathbf{y}$ , namely, the *weighted* and *anchored* Sobolev space  $\mathscr{W}_\gamma$ , which is a Hilbert space containing functions defined over  $U$ , with square integrable mixed first derivatives. More precisely, the norm is given by

$$\|F\|_{\mathscr{W}_\gamma} := \left( \sum_{|\mathbf{u}| < \infty} \frac{1}{\gamma_{\mathbf{u}}} \int_{[-\frac{1}{2}, \frac{1}{2}]^{|\mathbf{u}|}} \left| \frac{\partial^{|\mathbf{u}|} F}{\partial \mathbf{y}_{\mathbf{u}}}(\mathbf{y}_{\mathbf{u}}; 0) \right|^2 d\mathbf{y}_{\mathbf{u}} \right)^{1/2}, \quad (8)$$

where the sum is over all subsets  $\mathbf{u} \subset \mathbb{N}$  with finite cardinality  $|\mathbf{u}|$ ,  $\frac{\partial^{|\mathbf{u}|} F}{\partial \mathbf{y}_{\mathbf{u}}}$  denotes the mixed first derivative with respect to the variables  $y_j$  with  $j \in \mathbf{u}$ , and  $(\mathbf{y}_{\mathbf{u}}; 0)$  denotes the vector whose  $j$ th component is  $y_j$  if  $j \in \mathbf{u}$  and 0 if  $j \notin \mathbf{u}$ . The ‘‘anchor’’ in this case is  $(0, 0, \dots)$ , the center of the cube  $U$ .

Since our multi-level QMC-FE algorithm makes use of the FE solution of the truncated PDE problem to, say,  $s$  terms, we will consider also an  $s$ -dimensional variant of the space  $\mathscr{W}_\gamma$ , denoted by  $\mathscr{W}_{s,\gamma}$ , whose norm  $\|\cdot\|_{\mathscr{W}_{s,\gamma}}$  is defined by replacing the sum over all finite subsets  $\mathbf{u}$  in (8) by a sum over all subsets of the first  $s$  indices (i.e.,  $|\mathbf{u}| < \infty$  becomes  $\mathbf{u} \subseteq \{1, \dots, s\}$ ). For a function  $F$  that depends on infinitely many variables, if we define  $F^s(y_1, \dots, y_s) := F(y_1, \dots, y_s, 0, 0, \dots)$  by anchoring the components beyond dimension  $s$  at 0, then we have  $\|F^s\|_{\mathscr{W}_{s,\gamma}} = \|F^s\|_{\mathscr{W}_\gamma} \leq \|F\|_{\mathscr{W}_\gamma}$ .

Weighted spaces were first introduced by Sloan and Woźniakowski in [33], and by now there are many variants, see e.g. [12, 34]. As in [23], we have taken the cube to be centered at the origin (rather than the standard unit cube  $[0, 1]^s$ ), and the anchor is at the centre of the cube (rather than at a corner of the cube). Moreover, we have adopted ‘‘general weights’’: there is a weight parameter  $\gamma_{\mathbf{u}}$  associated with each group of variables  $\mathbf{y}_{\mathbf{u}} = (y_j)_{j \in \mathbf{u}}$  with indices belonging to the set  $\mathbf{u}$ , with the convention that  $\gamma_\emptyset = 1$ . Later we will focus on ‘‘POD weights’’, see (5). As in [23], these POD weights arise naturally from our analysis for the PDE application.

## 2.2 Parametric Weak Formulation

As in [23], we consider the following *parameter-dependent weak formulation of the parametric deterministic problem (1)*: for  $f \in V^*$  and  $\mathbf{y} \in U$ , find

$$u(\cdot, \mathbf{y}) \in V : \quad b(\mathbf{y}; u(\cdot, \mathbf{y}), v) = (f, v) \quad \forall v \in V, \quad (9)$$

where the parametric bilinear form  $b(\mathbf{y}; w, v)$  is given by

$$b(\mathbf{y}; w, v) := \int_D a(\mathbf{x}, \mathbf{y}) \nabla w(\mathbf{x}) \cdot \nabla v(\mathbf{x}) \, d\mathbf{x}, \quad \forall w, v \in V,$$

It follows from Assumption **(A2)** that the bilinear form is continuous and coercive on  $V \times V$ , and we may infer from the Lax-Milgram Lemma the existence of a unique solution to (9) satisfying the standard a-priori estimate. Moreover, additional regularity of the solution with respect to  $\mathbf{x}$  can be obtained under additional regularity assumptions on  $f$  and the coefficients  $a(\cdot, \mathbf{y})$ .

**Theorem 1 ([23, Theorems 3.1 and 4.1])** *Under Assumptions **(A1)** and **(A2)**, for every  $f \in V^*$  and every  $\mathbf{y} \in U$ , there exists a unique solution  $u(\cdot, \mathbf{y}) \in V$  of the parametric weak problem (9), which satisfies*

$$\|u(\cdot, \mathbf{y})\|_V \leq \frac{\|f\|_{V^*}}{a_{\min}}. \quad (10)$$

*If, in addition,  $f \in H^{-1+t}(D)$  for some  $0 \leq t \leq 1$ , and if Assumption **(A4)** holds, then there exists a constant  $C > 0$  such that for every  $\mathbf{y} \in U$ ,*

$$\|u(\cdot, \mathbf{y})\|_{Z^t} \leq C \|f\|_{H^{-1+t}(D)}, \quad (11)$$

*with the norm in  $Z^t$  defined by (7).*

## 2.3 Dimension Truncation

Next we summarize a result from [23] needed for estimating the dimension truncation error. Given  $s \in \mathbb{N}$  and  $\mathbf{y} \in U$ , we observe that truncating the sum in (2) at  $s$  terms is the same as anchoring or setting  $y_j = 0$  for  $j > s$ . With  $\{1 : s\}$  standing for  $\{1, \dots, s\}$ , we denote by  $u^s(\mathbf{x}, \mathbf{y}) := u(\mathbf{x}, (\mathbf{y}_{\{1:s\}}; \mathbf{0}))$  the solution of the parametric weak problem (9) corresponding to the parametric diffusion coefficient (2) when the sum is truncated after  $s$  terms. As observed in [23], it will be convenient for the regularity analysis of (1) and for the QMC error analysis to introduce

$$b_j := \frac{\|\psi_j\|_{L^\infty(D)}}{a_{\min}}, \quad j \geq 1. \quad (12)$$



**Theorem 2 ([23, Theorem 5.1])** *Under Assumptions (A1) and (A2), for every  $f \in V^*$ , every  $G \in V^*$ , every  $\mathbf{y} \in U$  and every  $s \in \mathbb{N}$ , the solution  $u^s(\cdot, \mathbf{y}) = u(\cdot, \mathbf{y}_{\{1:s\}}; 0)$  of the truncated parametric weak problem (9) satisfies, with  $b_j$  as defined in (12),*

$$\|u(\cdot, \mathbf{y}) - u^s(\cdot, \mathbf{y})\|_V \leq C \frac{\|f\|_{V^*}}{a_{\min}} \sum_{j \geq s+1} b_j$$

and

$$|I(G(u)) - I_s(G(u))| \leq \tilde{C} \frac{\|f\|_{V^*} \|G(\cdot)\|_{V^*}}{a_{\min}} \left( \sum_{j \geq s+1} b_j \right)^2 \quad (13)$$

for some constants  $C, \tilde{C} > 0$  independent of  $s$ ,  $f$  and  $G(\cdot)$ . In addition, if Assumptions (A3) and (A5) hold, then

$$\sum_{j \geq s+1} b_j \leq \min \left( \frac{1}{1/p - 1}, 1 \right) \left( \sum_{j \geq 1} b_j^p \right)^{1/p} s^{-(1/p-1)}. \quad (14)$$

## 2.4 Finite Element Discretization

Let us denote by  $\{V_h\}_h$  a one-parameter family of subspaces  $V_h \subset V$  of dimensions  $M_h < \infty$ . Under Assumption (A6), we think of the spaces  $V_h$  as spaces of continuous, piecewise-linear finite elements on a sequence of regular, simplicial meshes  $\mathcal{T}_h$  in  $D$  obtained from an initial, regular triangulation  $\mathcal{T}_0$  of  $D$  by recursive, uniform bisection of simplices. Then it is well known (see, e.g., [4]) that there exists a constant  $C > 0$  such that, as  $h \rightarrow 0$ , with the norm in  $Z^t$  defined by (7),

$$\inf_{v_h \in V_h} \|v - v_h\|_V \leq Ch^t \|v\|_{Z^t} \quad \text{for all } v \in Z^t, \quad 0 \leq t \leq 1.$$

For any  $\mathbf{y} \in U$ , we define the *parametric FE approximation*  $u_h(\cdot, \mathbf{y})$  as the FE solution of the parametric deterministic problem: for  $f \in V^*$  and  $\mathbf{y} \in U$ , find

$$u_h(\cdot, \mathbf{y}) \in V_h : \quad b(\mathbf{y}; u_h(\cdot, \mathbf{y}), v_h) = (f, v_h) \quad \forall v_h \in V_h.$$

Below we summarize the results from [23] regarding the FE error. We remark that, by considering the error in approximating a bounded linear functional,  $\mathcal{O}(h^2)$  convergence for  $f, G(\cdot) \in L^2(D)$  follows from an Aubin-Nitsche duality argument.

**Theorem 3 ([23, Theorems 7.1 and 7.2])** *Under Assumptions (A1), (A2), (A4), and (A6), for every  $f \in V^*$  and every  $\mathbf{y} \in U$ , the FE approximations  $u_h(\cdot, \mathbf{y})$  are stable in the sense that*

$$\|u_h(\cdot, \mathbf{y})\|_V \leq \frac{\|f\|_{V^*}}{a_{\min}}.$$

Moreover, for every  $f \in H^{-1+t}(D)$  with  $0 \leq t \leq 1$ , every  $G(\cdot) \in H^{-1+t'}$  with  $0 \leq t' \leq 1$ , and for every  $\mathbf{y} \in U$ , there hold the asymptotic convergence estimates as  $h \rightarrow 0$

$$\|u(\cdot, \mathbf{y}) - u_h(\cdot, \mathbf{y})\|_V \leq Ch^t \|u(\cdot, \mathbf{y})\|_{Z^t} \leq Ch^t \|f\|_{H^{-1+t}(D)} \quad (15)$$

and

$$|G(u(\cdot, \mathbf{y})) - G(u_h(\cdot, \mathbf{y}))| \leq \tilde{C} h^\tau \|f\|_{H^{-1+t}(D)} \|G(\cdot)\|_{H^{-1+t'}(D)}, \quad (16)$$

where  $0 \leq \tau := t + t' \leq 2$ , and where  $C, \tilde{C} > 0$  are independent of  $h$  and  $\mathbf{y}$ .

## 2.5 QMC Approximation

As in [23], in this paper we will focus on a family of QMC rules known as *randomly shifted lattice rules*. For an integral over the  $s$ -dimensional unit cube  $[-\frac{1}{2}, \frac{1}{2}]^s$ ,

$$I_s(F) := \int_{[-\frac{1}{2}, \frac{1}{2}]^s} F(\mathbf{y}) \, d\mathbf{y},$$

a realization of an  $N$ -point randomly shifted lattice rule takes the form

$$Q_{s,N}(\mathbf{\Delta}; F) := \frac{1}{N} \sum_{i=1}^N F\left(\text{frac}\left(\frac{i\mathbf{z}}{N} + \mathbf{\Delta}\right) - \left(\frac{1}{2}, \dots, \frac{1}{2}\right)\right),$$

where  $\mathbf{z} \in \mathbb{Z}^s$  is known as the *generating vector*, which is deterministic, while  $\mathbf{\Delta}$  is the *random shift* to be drawn from the uniform distribution on  $[0, 1]^s$ , and  $\text{frac}(\cdot)$  means to take the fractional part of each component in the vector. The subtraction by the vector  $(\frac{1}{2}, \dots, \frac{1}{2})$  describes the translation from the usual unit cube  $[0, 1]^s$  to  $[-\frac{1}{2}, \frac{1}{2}]^s$ . Good generating vectors  $\mathbf{z}$  for POD weights can be constructed using a *component-by-component algorithm*, at the cost of  $\mathcal{O}(N \log N s + N s^2)$  operations, such that the “shift averaged” *worst case error* in the weighted Sobolev space  $\mathcal{W}_{s,\boldsymbol{\gamma}}$  achieves a dimension-independent convergence rate close to  $\mathcal{O}(N^{-1})$ . Moreover, the implied constant in the big- $\mathcal{O}$  bound can be independent of  $s$  under appropriate conditions on the weights  $\gamma_u$ . A short summary of these results, together with references, can be found in [23, Section 2]. A more detailed survey can be found in [22]. For the purpose of this paper, we only need the following bound on the root-mean-square error.

**Theorem 4 ([23, Theorem 2.1])** *Let  $s, N \in \mathbb{N}$  be given, and assume  $F \in \mathcal{W}_{s,\boldsymbol{\gamma}}$  for a particular choice of weights  $\boldsymbol{\gamma} = (\gamma_u)$ . Then a randomly shifted lattice rule can be constructed using a component-by-component algorithm such that the root-mean-square error satisfies, for all  $\lambda \in (1/2, 1]$ ,*

$$\sqrt{\mathbb{E} [|I_s(F) - Q_{s,N}(\cdot; F)|^2]} \leq \left( \sum_{\emptyset \neq \mathbf{u} \subseteq \{1:s\}} \gamma_{\mathbf{u}}^\lambda [\rho(\lambda)]^{|\mathbf{u}|} \right)^{1/(2\lambda)} [\varphi(N)]^{-1/(2\lambda)} \|F\|_{\mathcal{W}_{s,\boldsymbol{\gamma}}},$$

where  $\mathbb{E}[\cdot]$  denotes the expectation with respect to the random shift which is uniformly distributed over  $[0, 1]^s$ ,  $\varphi(N) = |\{1 \leq z \leq N-1 : \gcd(z, N) = 1\}|$  denotes the Euler totient function,

$$\rho(\lambda) := \frac{2\zeta(2\lambda)}{(2\pi^2)^\lambda} + \frac{1}{12\lambda}, \quad (17)$$

and  $\zeta(x) = \sum_{k=1}^{\infty} k^{-x}$  denotes the Riemann zeta function.

A rate of convergence arbitrarily close to  $\mathcal{O}(N^{-1})$  comes from taking  $\lambda$  in the theorem close to  $1/2$ . However, note that  $\rho(\lambda) \rightarrow \infty$  as  $\lambda \rightarrow (1/2)_+$ , making the convergence of the sum over  $\mathbf{u}$  more and more problematic as  $\lambda$  comes closer to  $1/2$ . For that reason we shall leave  $\lambda$  as a free parameter in the subsequent discussion.

### 3 Multi-level QMC-FE Algorithm

#### 3.1 Formulation of the Multi-level QMC-FE Algorithm

We are now ready to formulate our multi-level QMC-FE algorithm for approximating the integral (3). Let

$$h_\ell = 2^{-\ell} h_0 \quad \text{for} \quad \ell = 0, 1, 2, \dots$$

We suppose that we are given a nested sequence  $\{V_{h_\ell}\}_{\ell \geq 0}$  of finite-dimensional subspaces of  $V$  of increasing dimension,

$$M_{h_0} < M_{h_1} < \dots < M_{h_\ell} := \dim(V_{h_\ell}) \asymp 2^{d\ell} \rightarrow \infty \quad \text{as} \quad \ell \rightarrow \infty,$$

where  $a_n \asymp b_n$  means there exist  $c_1, c_2 > 0$  such that  $c_1 b_n \leq a_n \leq c_2 b_n$ . In the multi-level method we specify a maximum level  $L$ , and with each level  $\ell = 0, \dots, L$  of (uniform) mesh refinement  $\mathcal{T}_{h_\ell}$  we associate a randomly shifted lattice rule  $Q_{s_\ell, N_\ell}$  which uses  $N_\ell$  points in  $s_\ell$  dimensions. We assume moreover that the sequence  $\{s_\ell\}_{\ell=0, \dots, L}$  of active dimensions is nondecreasing, i.e.,

$$s_0 \leq s_1 \leq \dots \leq s_\ell \leq s_L, \quad (18)$$

which implies that the corresponding sets of active coordinates are nested. To simplify the ensuing presentation, we write (with slight abuse of notation)

$$V_\ell \equiv V_{h_\ell}, \quad \mathcal{T}_\ell \equiv \mathcal{T}_{h_\ell}, \quad Q_\ell \equiv Q_{s_\ell, N_\ell}, \quad I_\ell \equiv I_{s_\ell}, \quad u_\ell \equiv u_{h_\ell}^{s_\ell}, \quad M_\ell \equiv M_{h_\ell}.$$

Here by  $u_{h_\ell}^{s_\ell}$  we mean the FE solution of the truncated problem with  $s_\ell$  terms in the expansion, which is the same as  $u_{h_\ell}(\mathbf{y}_{\{1:s_\ell\}}; 0)$ . For convenience we define  $u_{-1} := 0$ . Each lattice rule  $Q_\ell$  depends on a deterministic generating vector  $\mathbf{z}_\ell \in \mathbb{Z}^{s_\ell}$ , but we shall suppress this dependence in our notation. A realization of the lattice rule  $Q_\ell$  for a draw of the shift  $\mathbf{\Delta}_\ell \in [0, 1]^{s_\ell}$  applied to a function  $F$  will be denoted by  $Q_\ell(\mathbf{\Delta}_\ell; F)$ . The random shifts  $\mathbf{\Delta}_0, \dots, \mathbf{\Delta}_L$  are drawn independently from the uniform distribution on unit cubes of the appropriate dimension. With these notations, a single realization of our multi-level QMC-FE approximation of  $I(G(u))$  is given by

$$Q_*^L(\mathbf{\Delta}_*; G(u)) := \sum_{\ell=0}^L Q_\ell(\mathbf{\Delta}_\ell; G(u_\ell - u_{\ell-1})), \quad (19)$$

where  $\mathbf{\Delta}_* := (\mathbf{\Delta}_0, \dots, \mathbf{\Delta}_L)$  will be referred to as the ‘‘compound shift’’: it comprises all  $s_* := \sum_{\ell=0}^L s_\ell$  components of the random shifts  $\mathbf{\Delta}_\ell$ . Equivalently,  $\mathbf{\Delta}_*$  is drawn from the uniform distribution over  $[0, 1]^{s_*}$ .

The randomly shifted version of (19) that we use in practice makes use of  $m_\ell$  i.i.d. realizations of the level- $\ell$  shift  $\mathbf{\Delta}_\ell$ , thus takes the form

$$Q^L(G(u)) := \sum_{\ell=0}^L \frac{1}{m_\ell} \sum_{i=1}^{m_\ell} Q_\ell(\mathbf{\Delta}_\ell^{(i)}; G(u_\ell - u_{\ell-1})). \quad (20)$$

In the subsequent analysis we work with exact expectations of (19), but in the final section we return to (20), and there justify choosing  $m_\ell$  to be a fixed number independent of  $\ell$ .

### 3.2 Error Analysis of the Multi-level QMC-FE Algorithm

Using linearity of  $I$ ,  $I_\ell$ ,  $Q_\ell$  and  $G$ , we can express the error as

$$I(G(u)) - Q_*^L(\mathbf{\Delta}_*; G(u)) = I(G(u)) - \sum_{\ell=0}^L Q_\ell(\mathbf{\Delta}_\ell; G(u_\ell - u_{\ell-1})) = T_1 + T_2(\mathbf{\Delta}_*),$$

where

$$\begin{aligned} T_1 &:= I(G(u)) - \sum_{\ell=0}^L I_\ell(G(u_\ell - u_{\ell-1})), \\ T_2(\mathbf{\Delta}_*) &:= \sum_{\ell=0}^L (I_\ell - Q_\ell(\mathbf{\Delta}_\ell))(G(u_\ell - u_{\ell-1})), \end{aligned} \quad (21)$$

where we introduced the operator notation  $Q(\Delta)(F) := Q(\Delta; F)$ . Since a randomly shifted lattice rule is an unbiased estimator of the original integral, it follows that the mean-square error for our multi-level QMC-FE method, i.e., the expectation of the square error with respect to  $\mathbf{\Delta}_* \in [0, 1]^{s_*}$ , simplifies to

$$\mathbb{E}[|I(G(u)) - Q_*^L(\cdot; G(u))|^2] = T_1^2 + \mathbb{E}[T_2^2], \quad (22)$$

where the cross term vanishes due to  $\mathbb{E}[T_2] = 0$ , and we have

$$\mathbb{E}[T_2^2] = \sum_{\ell=0}^L \mathbb{E}[|(I_\ell - Q_\ell(\cdot))(G(u_\ell - u_{\ell-1}))|^2], \quad (23)$$

where the expectation inside the sum over index  $\ell$  is with respect to the random shift  $\mathbf{\Delta}_\ell \in [0, 1]^{s_\ell}$ .

First we estimate  $T_1$  given by (21). Since  $u_\ell - u_{\ell-1}$  only depends on the first  $s_\ell$  dimensions, we can replace  $I_\ell(G(u_\ell - u_{\ell-1}))$  by  $I(G(u_\ell - u_{\ell-1}))$ , and hence the expression (21) simplifies to

$$T_1 = I(G(u - u_L)) = I(G(u - u_{h_L})) + I(G(u_{h_L} - u_{h_L}^{s_L})).$$

Here  $u_{h_L} - u_{h_L}^{s_L}$  is the error that we incur in the FE approximation by omitting in the coefficient expansion (2) all terms with indices  $j > s_L$ . As we will show in Theorem 5 below, *this dimension truncation error vanishes for certain types of (multiresolution) coefficient expansion (2)*. To allow for this, we introduce a parameter  $\theta_L \in \{0, 1\}$ , and arrive at the estimate

$$\begin{aligned} |T_1| &\leq \sup_{\mathbf{y} \in U} |G(u(\cdot, \mathbf{y}) - u_{h_L}(\cdot, \mathbf{y}))| + \theta_L |I(G(u_{h_L} - u_{h_L}^{s_L}))| \\ &\leq Ch_L^\tau \|f\|_{H^{-1+\tau}(D)} \|G(\cdot)\|_{H^{-1+\tau'}(D)} + \theta_L \tilde{C} \frac{\|f\|_{V^*} \|G(\cdot)\|_{V^*}}{a_{\min}} \left( \sum_{j \geq s_L+1} b_j \right)^2, \end{aligned} \quad (24)$$

where for the first term we applied (16) from Theorem 3, and for the second term we used (13) from Theorem 2 but adapted to the FE solution  $u_{h_L}$  instead of  $u$ .

Next we estimate  $\mathbb{E}[T_2^2]$  given by (23). We have from Theorem 4 that

$$\mathbb{E}[T_2^2] \leq \sum_{\ell=0}^L \left( \sum_{\emptyset \neq u \subseteq \{1:s_\ell\}} \gamma_u^\lambda [\rho(\lambda)]^{|u|} \right)^{1/\lambda} [\varphi(N_\ell)]^{-1/\lambda} \|G(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}})\|_{\mathcal{W}_{s_\ell, \boldsymbol{\gamma}}}^2. \quad (25)$$

To estimate each term in (25) for  $\ell \neq 0$ , we write

$$\|G(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}})\|_{\mathcal{W}_{s_\ell, \boldsymbol{\gamma}}} \leq \|G(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_\ell})\|_{\mathcal{W}_{s_\ell, \boldsymbol{\gamma}}} + \|G(u_{h_{\ell-1}}^{s_\ell} - u_{h_{\ell-1}}^{s_{\ell-1}})\|_{\mathcal{W}_{s_\ell, \boldsymbol{\gamma}}}. \quad (26)$$

In §3.4 ahead, we bound the two terms in (26) separately, and then return to complete the error analysis in §3.5. Note that the second term in (26) vanishes if  $s_\ell = s_{\ell-1}$ . It also vanishes in the special case when, for all  $\ell \geq 1$  and an appropriately chosen increasing sequence  $s_\ell$ , we have  $u_{h_{\ell-1}}^{s_{\ell-1}} = u_{h_{\ell-1}}^{s_\ell} = u_{h_{\ell-1}}$ . This can happen when there is a special orthogonality property between the functions  $\psi_j$  in the representation (2) and the FE spaces  $V_\ell$ . We discuss this very important special case in the next subsection.

### 3.3 A Special Case with an Orthogonality Property

In this subsection we suppose that the sequence  $\psi_j$  has properties usually associated with a multiresolution analysis of  $L^2(D)$ , as shown in the Haar wavelet example below. For this purpose it is useful to relabel the basis set with a double index, as

$$\{\psi_j : j \geq 1\} = \{\psi_m^n : n \geq 0, m \in J_n\}, \quad (27)$$

where the first index  $n$  indicates the (multiresolution) level, and the second index  $m \in J_n$  indicates the location of a level- $n$  basis function within  $D$ , with  $J_n$  denoting the set of all location indices at level  $n$ . We suppose that all basis functions  $\psi_m^n$  at level  $n$  are piecewise polynomial functions on the triangulation  $\mathcal{T}_n$ , and have isotropic support whose diameter is of exact order  $h_n$ , implying  $|J_n| \asymp 2^{dn}$ .

**Definition 1** Let  $S^0(D, \mathcal{T})$  and  $S^1(D, \mathcal{T})$  be the subspaces defined by

$$\begin{aligned} S^0(D, \mathcal{T}) &:= \{v \in L^2(D) : v|_K \in P^0(K) \text{ for all } K \in \mathcal{T}\}, \\ S^1(D, \mathcal{T}) &:= \{v \in H_0^1(D) : v|_K \in P^1(K) \text{ for all } K \in \mathcal{T}\}, \end{aligned}$$

where  $P^r(K)$  denotes the space of polynomials of degree less than or equal to  $r$  on the element  $K$ . We say that the set  $\{\psi_m^n\}_{n \geq 0, m \in J_n}$  has the  $k$ -orthogonality property, for  $k \in \{1, 2\}$ , with respect to the triangulations  $\{\mathcal{T}_\ell : \ell \geq 0\}$  if for all  $\ell \geq 0$  we have

$$\int_D \psi_m^n(\mathbf{x}) z_\ell(\mathbf{x}) \, d\mathbf{x} = 0 \quad \text{for all } n \geq \ell + k, m \in J_n, \text{ and } z_\ell \in S^0(D, \mathcal{T}_\ell), \quad (28)$$

and  $\psi_m^n \in S^{k-1}(D, \mathcal{T}_{\ell+k-1})$  for all  $n \leq \ell + k - 1, m \in J_n$ , and  $\text{diam}(\text{supp}(\psi_m^n)) \asymp h_n$ .

A necessary condition for (28) to hold is that the functions  $\psi_m^n$  for  $n \geq k$  have the vanishing mean property, that is

$$\int_D \psi_m^n(\mathbf{x}) \, d\mathbf{x} = 0 \quad \text{for all } n \geq k \text{ and all } m \in J_n.$$

*Example 1 (Haar Wavelets)* We describe here the simplest case, of Haar wavelets for a one-dimensional domain  $D = [0, a]$ , with  $a$  some positive integer greater than or equal to 2. In the Haar wavelet case we may take, for  $m = 0, \dots, a - 1$ ,

$$\psi_m^0(x) := \begin{cases} 1 & \text{for } x \in [m, m + 1), \\ 0 & \text{otherwise,} \end{cases}$$

and for  $n \geq 1$ ,

$$\psi_m^n(x) := d_m^n \psi(2^n x - 2m), \quad m = 0, \dots, 2^{n-1}a - 1,$$

where  $d_m^n$  is a sequence of nonnegative scaling parameters,  $\psi(x)$  is 1 for  $x \in [0, 1)$ ,  $-1$  for  $x \in [1, 2)$ , and 0 otherwise. The family  $\{\psi_m^n\}$  forms an orthogonal basis of  $L^2([0, a])$  if  $d_m^n > 0$ . We remark that the choice  $d_m^n = 2^{(n-1)/2}$  which is well-known to imply orthonormality of the  $\psi_m^n$  in  $L^2([0, a])$  is inconsistent with **(A1)**, and is therefore excluded.

For the finite element space  $V_0$  we take the piecewise-linear functions vanishing at 0 and  $a$ . This space is spanned by the hat functions centered at  $1, 2, \dots, a - 1$ . The spaces  $V_\ell$  are then the piecewise-linear functions on  $[0, a]$  vanishing at 0 and  $a$ , spanned by the hat functions centered at multiples of  $2^{-\ell}$ . Correspondingly,  $\mathcal{T}_\ell$  is the mesh consisting of the multiples of  $2^{-\ell}$ , and the elements  $K_\ell$  are the intervals of length  $2^{-\ell}$  between the mesh points.

With this definition of  $\mathcal{T}_\ell$ , the multiresolution sequence  $\{\psi_m^n\}$  has the  $k$ -orthogonality property with respect to  $\mathcal{T}_\ell$  with  $k = 1$ , for all  $\ell \geq 0$ . For example, for  $\ell = 0$  and  $n = 1, m = 0$  we have, with  $z_0 \in S^0([0, a], \mathcal{T}_0)$  and  $c := z_0|_{[0, 1]}$ ,

$$\int_0^a \psi_0^1(x) z_0(x) dx = c \int_0^1 \psi_0^1(x) dx = c d_0^1 \int_0^1 \psi(2x) dx = 0.$$

Haar wavelets do not satisfy Assumption **(A4)**, since for **(A4)** to hold the basis functions  $\psi_m^n$  need to be Lipschitz continuous. A piecewise-linear  $k$ -orthogonal basis set with  $k = 2$  in dimension  $d = 1$  is constructed, for example, in [8]. For detailed constructions of  $k$ -orthogonality basis sets with  $k = 2$  and  $d > 1$ , see [8, 25]; for the case  $k = 1$  and  $d > 1$  see [2, Section 5].

In the following theorem, we show that there is *no truncation error at any level* for our multi-level algorithm under  $k$ -orthogonality if the dimension for truncation  $s_\ell$  is chosen appropriately at each level. To achieve this, we employ a one-to-one mapping of the indices between the functions  $\psi_j$  and  $\psi_m^n$  in (27): instead of ordering the functions as in Assumption **(A5)**, we index  $j$  according to a level-wise grouping so that the functions  $\{\psi_m^0\}_{m \in J_0}$  come before the functions  $\{\psi_m^1\}_{m \in J_1}$ , followed by the functions  $\{\psi_m^2\}_{m \in J_2}$ , and so on. Correspondingly, we employ the same index mapping between  $y_j$  and  $y_m^n$  for the components of  $\mathbf{y}$ .

**Theorem 5** *Let  $\{\psi_m^n : n \geq 0, m \in J_n\}$  be a multiresolution basis set for the domain  $D$ , with  $|J_n| \asymp 2^{dn}$ , which has the  $k$ -orthogonality property with  $k \in \{1, 2\}$  with respect to*

the triangulations  $\{\mathcal{T}_\ell : \ell \geq 0\}$ . Let  $\{\mathbf{y}_j : j \geq 1\} = \{y_m^n : n \geq 0, m \in J_n\}$  denote the corresponding parameters under the level-wise relabelling (27) so that the parametric coefficient in (2) can be represented in the form

$$a(\mathbf{x}, \mathbf{y}) = \bar{a}(\mathbf{x}) + \sum_{n=0}^{\infty} \sum_{m \in J_n} y_m^n \psi_m^n(\mathbf{x}).$$

Let

$$s_\ell := \sum_{n=0}^{\ell+k-1} |J_n|. \quad (29)$$

Then  $s_\ell \asymp 2^{d\ell} \asymp M_{h_\ell}$ , and for all  $\ell \geq 0$  we have

$$u_{h_\ell} = u_{h_\ell}^{s_\ell}. \quad (30)$$

Moreover, the cost for exact evaluation of the Finite Element stiffness matrix for the parametric coefficient  $a(\mathbf{x}, \mathbf{y})$  at meshlevel  $\ell \geq 0$  for any given  $\mathbf{y} \in U$  is  $\mathcal{O}(M_{h_\ell} \log(M_{h_\ell}))$  operations.

*Proof* There holds  $\nabla V_\ell \subseteq S^0(D, \mathcal{T}_\ell)^d$  for all  $\ell \geq 0$ . Thus, for all  $\ell \geq 0$  and for every  $v_\ell, w_\ell \in V_\ell$ , we have  $\nabla w_\ell \cdot \nabla v_\ell \in S^0(D, \mathcal{T}_\ell)$ . The  $k$ -orthogonality property (28) therefore implies for all  $\ell \geq 0$  and for all  $v_\ell, w_\ell \in V_\ell$

$$\begin{aligned} b(\mathbf{y}; w_\ell, v_\ell) &= \int_D \left( \bar{a}(\mathbf{x}) + \sum_{n=0}^{\infty} \sum_{m \in J_n} y_m^n \psi_m^n(\mathbf{x}) \right) \nabla w_\ell \cdot \nabla v_\ell \, d\mathbf{x} \\ &= \int_D \left( \bar{a}(\mathbf{x}) + \sum_{n=0}^{\ell+k-1} \sum_{m \in J_n} y_m^n \psi_m^n(\mathbf{x}) \right) \nabla w_\ell \cdot \nabla v_\ell \, d\mathbf{x} \\ &= b(\mathbf{y}_{\{1:s_\ell\}}; w_\ell, v_\ell). \end{aligned} \quad (31)$$

The assertion (30) then follows from the uniqueness of the FE solutions.

To show the assertion on the cost, for given  $\mathbf{y}$  we denote by  $\mathbf{B}^\ell(\mathbf{y})$  the  $M_\ell \times M_\ell$  stiffness matrix of the parametric bilinear form  $b(\mathbf{y}; \cdot, \cdot)$ , restricted to  $V_\ell \times V_\ell$ , where  $V_\ell = \text{span}\{\phi_i^\ell : 1 \leq i \leq M_\ell\}$ , with  $\phi_i^\ell$  denoting the nodal hat basis functions of  $S^1(D, \mathcal{T}_\ell)$ . By  $k$ -orthogonality of the  $\psi_m^n$ , we have (31), and for each  $1 \leq i, i' \leq M_\ell = \dim(V_\ell) = \mathcal{O}(2^{d\ell})$  there holds

$$\mathbf{B}^\ell(\mathbf{y})_{i i'} = b(\mathbf{y}_{\{1:s_\ell\}}; \phi_i^\ell, \phi_{i'}^\ell) = \int_D (P_{\ell+k-1} a(\mathbf{x}, \mathbf{y})) \nabla \phi_i^\ell \cdot \nabla \phi_{i'}^\ell \, d\mathbf{x}, \quad (32)$$

where  $P_{\ell+k-1} a(\mathbf{x}, \mathbf{y})$  denotes the truncated expression for  $a(\mathbf{x}, \mathbf{y})$  appearing in (31). The matrix  $\mathbf{B}^\ell(\mathbf{y})$  is sparse: it has, due to the local support of the hat functions  $\phi_i^\ell$  and due to the construction of the sequence  $\{\mathcal{T}_\ell\}_{\ell \geq 0}$  of meshes, at most  $\mathcal{O}(M_\ell)$  nonvanishing entries (32).

Now consider the cost for the *exact evaluation* of any matrix entry  $(\mathbf{B}^\ell(\mathbf{y}))_{i i'} \neq 0$ . Given  $\ell, i, i'$ , and for a given  $n \leq \ell + k - 1$ , it follows from the assumption on the support of  $\psi_m^n$  that there are only  $\mathcal{O}(1)$  many functions  $\psi_m^n$  such that  $\int_D \psi_m^n(\mathbf{x}) \nabla \phi_i^\ell \cdot \nabla \phi_{i'}^\ell \, d\mathbf{x} \neq 0$ . Thus the cost for evaluating  $(\mathbf{B}^\ell(\mathbf{y}))_{i i'} \neq 0$  is  $\mathcal{O}(\ell + k - 1)$ , which yields that the total cost for evaluating the sparse matrix is  $\mathcal{O}(M_\ell \ell) = \mathcal{O}(M_\ell \log(M_\ell))$  operations.  $\square$

### 3.4 Key Results

In the error analysis of the (single level) QMC-FE method, we established in [23] regularity results for the parametric solutions. In the present multi-level QMC-FE error analysis, we first establish stronger regularity of the PDE solution simultaneously with respect to both  $\mathbf{x}$  and  $\mathbf{y}$ . The result shown is actually more general than required in this paper: our result covers partial derivatives of arbitrary order. To state the result, we introduce further notation: for  $\mathbf{v} = (v_j)_{j \geq 1} \in \mathbb{N}_0^{\mathbb{N}}$ , where  $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$ , we define  $|\mathbf{v}| := v_1 + v_2 + \dots$ , and we refer to  $\mathbf{v}$  as a “multi-index” and  $|\mathbf{v}|$  as the “length” of  $\mathbf{v}$ . By

$$\mathfrak{F} := \{\mathbf{v} \in \mathbb{N}_0^{\mathbb{N}} : |\mathbf{v}| < \infty\}$$

we denote the (countable) set of all “finitely supported” multi-indices (i.e., sequences of nonnegative integers for which only finitely many entries are nonzero). For  $\mathbf{v} \in \mathfrak{F}$  we denote the partial derivative of order  $\mathbf{v} \in \mathfrak{F}$  of  $u$  with respect to  $\mathbf{y}$  by

$$\partial_{\mathbf{y}}^{\mathbf{v}} u := \frac{\partial^{|\mathbf{v}|}}{\partial y_1^{v_1} \partial y_2^{v_2} \dots} u.$$

**Theorem 6** *Under Assumptions (A1) and (A2), for every  $f \in V^*$ , every  $\mathbf{y} \in U$  and every  $\mathbf{v} \in \mathfrak{F}$ , the solution  $u(\cdot, \mathbf{y})$  of the parametric weak problem (9) satisfies*

$$\|\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})\|_V \leq |\mathbf{v}|! \left( \prod_{j \geq 1} b_j^{v_j} \right) \frac{\|f\|_{V^*}}{a_{\min}}, \quad (33)$$

where  $b_j$  is as defined in (12). If, in addition,  $f \in H^{-1+t}(D)$  for some  $0 \leq t \leq 1$ , and if Assumption (A4) holds, then for every  $\kappa \in (0, 1]$  there holds

$$\|\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})\|_{\mathcal{Z}^t} \leq C |\mathbf{v}|! \left( \prod_{j \geq 1} \bar{b}_j^{v_j} \right) \|f\|_{H^{-1+t}(D)}, \quad (34)$$

where

$$\bar{b}_j := b_j + \kappa C_t (\|\nabla \psi_j\|_{L^\infty(D)} + B \|\psi_j\|_{L^\infty(D)}), \quad j \geq 1, \quad (35)$$

and the constants  $B$  and  $C_t$  are, for  $0 \leq t \leq 1$ , defined by

$$B := \frac{1}{a_{\min}} \sup_{\mathbf{z} \in U} \|\nabla a(\cdot, \mathbf{z})\|_{L^\infty(D)} < \infty, \quad C_t := \sup_{w \in L^2(D)} \frac{\|w\|_{H^{-1+t}(D)}}{\|w\|_{L^2(D)}} < \infty. \quad (36)$$

In (34) we have  $C \leq \bar{C} \kappa^{-1}$  with  $\bar{C} > 0$  independent of  $\kappa$ .

*Proof* Assertion (33) was proved in [6, Theorem 4.3]. The proof there was based on the observation that, for every  $v \in V$ ,  $\mathbf{y} \in U$  and  $\mathbf{v} \in \mathfrak{F}$  with  $|\mathbf{v}| \neq 0$ , (9) implies the recurrence

$$(a(\cdot, \mathbf{y}) \nabla(\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})), \nabla v) + \sum_{j \in \text{supp}(\mathbf{v})} v_j \left( \psi_j \nabla(\partial_{\mathbf{y}}^{\mathbf{v}-\mathbf{e}_j} u(\cdot, \mathbf{y})), \nabla v \right) = 0, \quad (37)$$



where  $\mathbf{e}_j \in \mathfrak{F}$  denotes the multiindex with entry 1 in position  $j$  and zeros elsewhere, and where  $\text{supp}(\mathbf{v}) := \{j \in \mathbb{N} : v_j \neq 0\}$  denotes the ‘‘support’’ of  $\mathbf{v}$ . Taking  $v(\mathbf{x}) = \partial_{\mathbf{y}}^{\mathbf{v}} u(\mathbf{x}, \mathbf{y}) \in V$  in (37) leads to

$$\|\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})\|_V \leq \sum_{j \in \text{supp}(\mathbf{v})} v_j b_j \|\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})\|_V, \quad (38)$$

from which (33) follows by induction.

Assertion (34) was proved in [6, Theorem 8.2] for the case  $t = 1$ . For completeness we provide a proof for general  $t$  here. We proceed once more by induction. The case  $|\mathbf{v}| = 0$  is precisely (11) and is already proved in [23, Theorem 4.1]. To obtain the bounds for  $|\mathbf{v}| \neq 0$ , we observe that, trivially, for every  $\mathbf{v} \in \mathfrak{F}$  and for every  $\mathbf{y} \in U$ , the function  $\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})$  is the solution of the Dirichlet problem

$$-\nabla \cdot (a(\cdot, \mathbf{y}) \nabla (\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y}))) = -g_{\mathbf{v}}(\cdot, \mathbf{y}) \quad \text{in } D, \quad \partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})|_{\partial D} = 0, \quad (39)$$

with

$$g_{\mathbf{v}}(\cdot, \mathbf{y}) := \nabla \cdot (a(\cdot, \mathbf{y}) \nabla (\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y}))) = \nabla a(\cdot, \mathbf{y}) \cdot \nabla (\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})) + a(\cdot, \mathbf{y}) \Delta (\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})).$$

Here, we used the identity

$$\nabla \cdot (\alpha(\mathbf{x}) \nabla w(\mathbf{x})) = \alpha(\mathbf{x}) \Delta w(\mathbf{x}) + \nabla \alpha(\mathbf{x}) \cdot \nabla w(\mathbf{x}), \quad (40)$$

which is valid for  $\alpha \in W^{1,\infty}(D)$  and for any  $w \in V$  such that  $\Delta w \in L^2(D)$ .

The assertion (34) will follow from (11), which implies for the solution of problem (39) the bound

$$\|\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})\|_{Z^t} \leq C \|g_{\mathbf{v}}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)}. \quad (41)$$

It remains to establish bounds for  $\|g_{\mathbf{v}}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)}$ . We recast (37) in strong form and obtain from (39), for every  $\mathbf{y} \in U$  and for every  $v \in H^{1-t}(D)$ ,

$$\begin{aligned} |(g_{\mathbf{v}}(\cdot, \mathbf{y}), v)| &= |(\nabla \cdot (a(\cdot, \mathbf{y}) \nabla (\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y}))), v)| \\ &= \left| \sum_{j \in \text{supp}(\mathbf{v})} v_j \left( \nabla \psi_j \cdot \nabla (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})) + \psi_j \Delta (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})) \right), v \right| \\ &\leq \sum_{j \in \text{supp}(\mathbf{v})} v_j \left\| \nabla \psi_j(\cdot) \cdot \nabla (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})) + \psi_j(\cdot) \Delta (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})) \right\|_{H^{-1+t}(D)} \|v\|_{H^{1-t}(D)}. \end{aligned}$$

Dividing by  $\|v\|_{H^{1-t}(D)}$  and taking the supremum over all  $v \in H^{1-t}(D)$  yields

$$\begin{aligned} \|g_{\mathbf{v}}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)} &\leq \sum_{j \in \text{supp}(\mathbf{v})} v_j \left( \|\nabla \psi_j\|_{L^\infty(D)} \left\| \nabla (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})) \right\|_{H^{-1+t}(D)} \right. \\ &\quad \left. + \|\psi_j\|_{L^\infty(D)} \left\| \Delta (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})) \right\|_{H^{-1+t}(D)} \right). \quad (42) \end{aligned}$$

To bound the second term on the right-hand side of (42), we write (39) with  $\mathbf{v} - \mathbf{e}_j$  in place of  $\mathbf{v}$ , for every  $\mathbf{y} \in U$ , in the form

$$-a(\cdot, \mathbf{y}) \Delta (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})) = \nabla a(\cdot, \mathbf{y}) \cdot \nabla (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})) - g_{\mathbf{v} - \mathbf{e}_j}(\cdot, \mathbf{y}), \quad (43)$$

using again (40). This implies, for every  $\mathbf{y} \in U$ , the estimate

$$\begin{aligned} \|\Delta (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y}))\|_{H^{-1+t}(D)} &\leq \frac{1}{a_{\min}} \|\text{RHS of (43)}\|_{H^{-1+t}(D)} \\ &\leq \frac{1}{a_{\min}} \left[ \left( \sup_{\mathbf{z} \in U} \|\nabla a(\cdot, \mathbf{z})\|_{L^\infty(D)} \right) \|\nabla (\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y}))\|_{H^{-1+t}(D)} + \|g_{\mathbf{v} - \mathbf{e}_j}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)} \right] \\ &\leq BC_t \|\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})\|_V + \frac{1}{a_{\min}} \|g_{\mathbf{v} - \mathbf{e}_j}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)}, \end{aligned}$$

where  $B$  and  $C_t$  are as in (36). We insert this bound into (42) to obtain

$$\begin{aligned} \|g_{\mathbf{v}}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)} &\leq \sum_{j \in \text{supp}(\mathbf{v})} \nu_j \left[ C_t (\|\nabla \psi_j\|_{L^\infty(D)} + B \|\psi_j\|_{L^\infty(D)}) \|\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})\|_V \right. \\ &\quad \left. + b_j \|g_{\mathbf{v} - \mathbf{e}_j}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)} \right]. \quad (44) \end{aligned}$$

This recursive estimate for  $\|g_{\mathbf{v}}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)}$  has structure which is similar to the bound (38) for  $\|\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})\|_V$ . We therefore multiply (44) by  $\kappa > 0$  and add it to (38) to obtain

$$\begin{aligned} &\|\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})\|_V + \kappa \|g_{\mathbf{v}}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)} \\ &\leq \sum_{j \in \text{supp}(\mathbf{v})} \nu_j b_j \left[ \|\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})\|_V + \kappa \|g_{\mathbf{v} - \mathbf{e}_j}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)} \right] \\ &\quad + \sum_{j \in \text{supp}(\mathbf{v})} \nu_j \kappa C_t (\|\nabla \psi_j\|_{L^\infty(D)} + B \|\psi_j\|_{L^\infty(D)}) \|\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})\|_V \\ &\leq \sum_{j \in \text{supp}(\mathbf{v})} \nu_j \bar{b}_j \left[ \|\partial_{\mathbf{y}}^{\mathbf{v} - \mathbf{e}_j} u(\cdot, \mathbf{y})\|_V + \kappa \|g_{\mathbf{v} - \mathbf{e}_j}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)} \right], \quad (45) \end{aligned}$$

where  $\bar{b}_j$  is as in (35). By Assumption (A4), we have  $\sum_{j \geq 1} \bar{b}_j < \infty$  for any choice of  $\kappa > 0$  and for any  $B$ .

To establish (34) it remains to observe that the estimate (45) has the same structure as (38), with the sequence  $\{\bar{b}_j\}$  in place of  $\{b_j\}$ . For  $|\mathbf{v}| = 0$ , we find using (10) of Theorem 1 and  $g_0 = -f$  that

$$\|u(\cdot, \mathbf{y})\|_V + \kappa \|g_0\|_{H^{-1+t}(D)} \leq \frac{1}{a_{\min}} \|f\|_{V^*} + \kappa \|f\|_{H^{-1+t}(D)}.$$

The same induction argument used to establish (33) applied to the recursive estimate (45) implies for all  $\mathbf{v} \in \mathfrak{F}$ , for every  $\mathbf{y} \in U$  and for every  $\kappa \in (0, 1]$

$$\begin{aligned} \kappa \|g_{\mathbf{v}}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)} &\leq \|\partial_{\mathbf{y}}^{\mathbf{v}} u(\cdot, \mathbf{y})\|_V + \kappa \|g_{\mathbf{v}}(\cdot, \mathbf{y})\|_{H^{-1+t}(D)} \\ &\leq |\mathbf{v}|! \left( \prod_{j \geq 1} \bar{b}_j^{\nu_j} \right) \left( \frac{\tilde{C}_t}{a_{\min}} + \kappa \right) \|f\|_{H^{-1+t}(D)}, \end{aligned}$$

where  $\tilde{C}_t := \sup_{w \in H^{-1+t}(D)} (\|w\|_{H^{-1}(D)} / \|w\|_{H^{-1+t}(D)}) < \infty$ . Now (34) follows from (41).  $\square$

To bound the first term in (26) we need the following result.

**Theorem 7** *Under Assumptions (A1), (A2), (A4), and (A6), for every  $f \in H^{-1+t}(D)$  with  $0 \leq t \leq 1$ , every  $G(\cdot) \in H^{-1+t'}(D)$  with  $0 \leq t' \leq 1$ , every  $\kappa \in (0, 1]$ , and every  $s \in \mathbb{N}$ , we have*

$$\begin{aligned} & \|G(u^s - u_h^s)\|_{\mathcal{W}_{s,\gamma}} \\ & \leq Ch^\tau a_{\max} \|f\|_{H^{-1+t}(D)} \|G(\cdot)\|_{H^{-1+t'}(D)} \left( \sum_{\mathbf{u} \subseteq \{1:s\}} \frac{[(|\mathbf{u}| + 1)!]^2 \prod_{j \in \mathbf{u}} \bar{b}_j^2}{\gamma_{\mathbf{u}}} \right)^{1/2}, \end{aligned}$$

where  $0 \leq \tau := t + t' \leq 2$ , where  $\bar{b}_j$  is defined in (35), and where the constant  $C > 0$  is independent of  $s$ .

*Proof* Let  $g \in H^{-1+t'}(D)$  denote the representer of  $G(\cdot) \in H^{-1+t'}(D)$ . For all  $\mathbf{y} \in U$ , we define  $v^g(\cdot, \mathbf{y}) \in V$  and  $v_h^g(\cdot, \mathbf{y}) \in V_h$  by

$$b(\mathbf{y}; w, v^g(\cdot, \mathbf{y})) = (g, w) \quad \forall w \in V, \quad (46)$$

$$b(\mathbf{y}; w_h, v_h^g(\cdot, \mathbf{y})) = (g, w_h) \quad \forall w_h \in V_h. \quad (47)$$

Taking  $w = u(\cdot, \mathbf{y}) - u_h(\cdot, \mathbf{y})$ , we have

$$\begin{aligned} G(u(\cdot, \mathbf{y}) - u_h(\cdot, \mathbf{y})) &= (g, u(\cdot, \mathbf{y}) - u_h(\cdot, \mathbf{y})) = b(\mathbf{y}; u(\cdot, \mathbf{y}) - u_h(\cdot, \mathbf{y}), v^g(\cdot, \mathbf{y})) \\ &= b(\mathbf{y}; u(\cdot, \mathbf{y}) - u_h(\cdot, \mathbf{y}), v^g(\cdot, \mathbf{y}) - v_h^g(\cdot, \mathbf{y})), \end{aligned}$$

where in the last step we used Galerkin orthogonality  $b(\mathbf{y}; u(\cdot, \mathbf{y}) - u_h(\cdot, \mathbf{y}), v_h^g(\cdot, \mathbf{y})) = 0$ .

Using the definitions of the bilinear form  $b(\mathbf{y}; \cdot, \cdot)$  and the norm  $\|\cdot\|_{\mathcal{W}_{s,\gamma}}$ , we obtain

$$\|G(u^s - u_h^s)\|_{\mathcal{W}_{s,\gamma}} = \left( \sum_{\mathbf{u} \subseteq \{1:s\}} \gamma_{\mathbf{u}}^{-1} \int_{[-\frac{1}{2}, \frac{1}{2}]^{|\mathbf{u}|}} \left| \int_D r_{\mathbf{u}}(\mathbf{x}, (\mathbf{y}_{\mathbf{u}}; 0)) d\mathbf{x} \right|^2 d\mathbf{y}_{\mathbf{u}} \right)^{1/2}, \quad (48)$$

where

$$r_{\mathbf{u}}(\mathbf{x}, \mathbf{y}) := \frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{y}_{\mathbf{u}}} \left( a(\mathbf{x}, \mathbf{y}) \nabla(u - u_h)(\mathbf{x}, \mathbf{y}) \cdot \nabla(v^g - v_h^g)(\mathbf{x}, \mathbf{y}) \right).$$

For the remainder of this proof, we will use the short-hand notation  $\partial_{\mathbf{u}}$  for the mixed first partial derivatives with respect to the variables  $y_j$  for  $j \in \mathbf{u}$ . We will also omit  $\mathbf{x}$  and  $\mathbf{y}$  in many places. From the special form of  $a(\mathbf{x}, \mathbf{y})$  we see that

$$\begin{aligned} r_{\mathbf{u}}(\mathbf{x}, \mathbf{y}) &= a(\mathbf{x}, \mathbf{y}) \partial_{\mathbf{u}} \left( \nabla(u - u_h) \cdot \nabla(v^g - v_h^g) \right) \\ &\quad + \sum_{k \in \mathbf{u}} \psi_k(\mathbf{x}) \partial_{\mathbf{u} \setminus \{k\}} \left( \nabla(u - u_h) \cdot \nabla(v^g - v_h^g) \right) \\ &= a(\mathbf{x}, \mathbf{y}) \sum_{\mathbf{v} \subseteq \mathbf{u}} \nabla \partial_{\mathbf{v}}(u - u_h) \cdot \nabla \partial_{\mathbf{u} \setminus \mathbf{v}}(v^g - v_h^g) \\ &\quad + \sum_{k \in \mathbf{u}} \psi_k(\mathbf{x}) \sum_{\mathbf{v} \subseteq \mathbf{u} \setminus \{k\}} \nabla \partial_{\mathbf{v}}(u - u_h) \cdot \nabla \partial_{(\mathbf{u} \setminus \{k\}) \setminus \mathbf{v}}(v^g - v_h^g), \end{aligned}$$

where in both terms we used the product rule  $\partial_{\mathbf{u}}(AB) = \sum_{\mathbf{v} \subseteq \mathbf{u}} (\partial_{\mathbf{v}}A)(\partial_{\mathbf{u} \setminus \mathbf{v}}B)$ . Thus

$$\begin{aligned} \left| \int_D r_{\mathbf{u}}(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} \right| &\leq a_{\max} \sum_{\mathbf{v} \subseteq \mathbf{u}} \|\partial_{\mathbf{v}}(u - u_h)\|_V \|\partial_{\mathbf{u} \setminus \mathbf{v}}(v^g - v_h^g)\|_V \\ &\quad + \sum_{k \in \mathbf{u}} \|\psi_k\|_{L^\infty(D)} \sum_{\mathbf{v} \subseteq \mathbf{u} \setminus \{k\}} \|\partial_{\mathbf{v}}(u - u_h)\|_V \|\partial_{(\mathbf{u} \setminus \{k\}) \setminus \mathbf{v}}(v^g - v_h^g)\|_V. \end{aligned} \quad (49)$$

Denoting by  $\mathcal{I} : V \rightarrow V$  the identity operator and by  $\mathcal{P}_h : V \rightarrow V_h$  the corresponding FE projection, we can write

$$\begin{aligned} \|\partial_{\mathbf{v}}(u - u_h)\|_V &= \|\partial_{\mathbf{v}}(\mathcal{I} - \mathcal{P}_h)u\|_V = \|(\mathcal{I} - \mathcal{P}_h)(\partial_{\mathbf{v}}u)\|_V \\ &\leq Ch^t \|\partial_{\mathbf{v}}u\|_{Z^t} \leq Ch^t \|f\|_{H^{-1+t}(D)} |\mathbf{v}|! \prod_{j \in \mathbf{v}} \bar{b}_j, \end{aligned} \quad (50)$$

where the first inequality follows from (15) in Theorem 3, and the second inequality follows from (34) in Theorem 6. Throughout,  $C > 0$  denotes a generic constant. Similarly, it follows from (46) and (47) that

$$\begin{aligned} \|\partial_{\mathbf{u} \setminus \mathbf{v}}(v^g - v_h^g)\|_V &= \|\partial_{\mathbf{u} \setminus \mathbf{v}}(\mathcal{I} - \mathcal{P}_h)v^g\|_V = \|(\mathcal{I} - \mathcal{P}_h)(\partial_{\mathbf{u} \setminus \mathbf{v}}v^g)\|_V \\ &\leq Ch^{t'} \|\partial_{\mathbf{u} \setminus \mathbf{v}}v^g\|_{Z^{t'}} \leq Ch^{t'} \|g\|_{H^{-1+t'}(D)} |\mathbf{u} \setminus \mathbf{v}|! \prod_{j \in \mathbf{u} \setminus \mathbf{v}} \bar{b}_j. \end{aligned} \quad (51)$$

Using (50) and (51), together with the identity  $\sum_{\mathbf{v} \subseteq \mathbf{u}} |\mathbf{v}|! |\mathbf{u} \setminus \mathbf{v}|! = (|\mathbf{u}| + 1)!$ , we obtain from (49)

$$\begin{aligned} \left| \int_D r_{\mathbf{u}}(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} \right| &\leq Ch^{t+t'} a_{\max} \|f\|_{H^{-1+t}(D)} \|g\|_{H^{-1+t'}(D)} (|\mathbf{u}| + 1)! \prod_{j \in \mathbf{u}} \bar{b}_j \\ &\quad + Ch^{t+t'} \|f\|_{H^{-1+t}(D)} \|g\|_{H^{-1+t'}(D)} \sum_{k \in \mathbf{u}} \|\psi_k\|_{L^\infty(D)} |\mathbf{u}|! \prod_{j \in \mathbf{u} \setminus \{k\}} \bar{b}_j \\ &\leq Ch^{t+t'} a_{\max} \|f\|_{H^{-1+t}(D)} \|G(\cdot)\|_{H^{-1+t'}(D)} (|\mathbf{u}| + 1)! \prod_{j \in \mathbf{u}} \bar{b}_j, \end{aligned}$$

where we used the estimate  $\|\psi_k\|_{L^\infty(D)} = a_{\min} b_k \leq a_{\max} \bar{b}_k$ . Substituting this estimate into (48) completes the proof.  $\square$

As we remarked earlier, if  $k$ -orthogonality (28) does not hold and if  $s_\ell > s_{\ell-1}$ , the second term in (26) is generally nonzero. We estimate it in the following result.

**Theorem 8** *Under Assumptions (A1) and (A2), for every  $f \in V^*$ , every  $G(\cdot) \in V^*$ , every  $h > 0$ , and every  $\ell \geq 1$ ,*

$$\begin{aligned} &\|G(u_h^{s_\ell} - u_h^{s_{\ell-1}})\|_{\mathcal{W}_{s_\ell, \mathcal{I}}} \\ &\leq \frac{a_{\max} \|f\|_{V^*} \|G(\cdot)\|_{V^*}}{a_{\min}^2} \left( \sum_{j=s_{\ell-1}+1}^{s_\ell} b_j \right) \left( \sum_{\mathbf{u} \subseteq \{1:s_\ell\}} \frac{[(|\mathbf{u}| + 1)!]^2 \prod_{j \in \mathbf{u}} b_j^2}{\gamma_{\mathbf{u}}} \right)^{1/2}, \end{aligned}$$

where  $b_j$  is defined in (12).

Note that if Assumptions **(A3)** and **(A5)** hold, then from (14) we have  $\sum_{j=s_{\ell-1}+1}^{s_\ell} b_j = \mathcal{O}(s_{\ell-1}^{-(1/p-1)})$ .

*Proof* We follow a similar line of argument to the proof of Theorem 7. Let  $g \in V^*$  denote the representer of  $G(\cdot) \in V$ . For all  $\mathbf{y} \in U$ , we define  $v_h^g(\cdot, \mathbf{y}) \in V_h$  as in (47). Taking  $w_h = u_h^{s_\ell}(\cdot, \mathbf{y}) - u_h^{s_{\ell-1}}(\cdot, \mathbf{y})$  in (47), we have

$$\begin{aligned} G(u_h^{s_\ell}(\cdot, \mathbf{y}) - u_h^{s_{\ell-1}}(\cdot, \mathbf{y})) &= (g, u_h^{s_\ell}(\cdot, \mathbf{y}) - u_h^{s_{\ell-1}}(\cdot, \mathbf{y})) \\ &= b(\mathbf{y}; u_h^{s_\ell}(\cdot, \mathbf{y}) - u_h^{s_{\ell-1}}(\cdot, \mathbf{y}), v_h^g(\cdot, \mathbf{y})). \end{aligned}$$

Using the definitions of the bilinear form  $b(\mathbf{y}; \cdot, \cdot)$  and the norm  $\|\cdot\|_{\mathcal{W}_{s_\ell, \mathbf{y}}}$ , we obtain

$$\|G(u_h^{s_\ell} - u_h^{s_{\ell-1}})\|_{\mathcal{W}_{s_\ell, \mathbf{y}}} = \left( \sum_{\mathbf{u} \subseteq \{1, \dots, s_\ell\}} \gamma_{\mathbf{u}}^{-1} \int_{[-\frac{1}{2}, \frac{1}{2}]^{|\mathbf{u}|}} \left| \int_D \tilde{r}_{\mathbf{u}}(\mathbf{x}, (\mathbf{y}_{\mathbf{u}}; 0)) \, d\mathbf{x} \right|^2 d\mathbf{y}_{\mathbf{u}} \right)^{1/2}, \quad (52)$$

where

$$\tilde{r}_{\mathbf{u}}(\mathbf{x}, \mathbf{y}) := \frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{y}_{\mathbf{u}}} \left( a(\mathbf{x}, \mathbf{y}) \nabla(u_h^{s_\ell} - u_h^{s_{\ell-1}})(\mathbf{x}, \mathbf{y}) \cdot \nabla v_h^g(\mathbf{x}, \mathbf{y}) \right).$$

As in the proof of Theorem 7, we will use the short-hand notation  $\partial_{\mathbf{u}}$  for the mixed first partial derivatives with respect to the variables  $y_j$  for  $j \in \mathbf{u}$ , and we will also omit  $\mathbf{x}$  and  $\mathbf{y}$  in many places below. From the special form of  $a(\mathbf{x}, \mathbf{y})$  we see that

$$\begin{aligned} \tilde{r}_{\mathbf{u}}(\mathbf{x}, \mathbf{y}) &= a(\mathbf{x}, \mathbf{y}) \partial_{\mathbf{u}} \left( \nabla(u_h^{s_\ell} - u_h^{s_{\ell-1}}) \cdot \nabla v_h^g \right) + \sum_{k \in \mathbf{u}} \psi_k(\mathbf{x}) \partial_{\mathbf{u} \setminus \{k\}} \left( \nabla(u_h^{s_\ell} - u_h^{s_{\ell-1}}) \cdot \nabla v_h^g \right) \\ &= a(\mathbf{x}, \mathbf{y}) \sum_{\mathbf{v} \subseteq \mathbf{u}} \nabla \partial_{\mathbf{v}}(u_h^{s_\ell} - u_h^{s_{\ell-1}}) \cdot \nabla \partial_{\mathbf{u} \setminus \mathbf{v}} v_h^g \\ &\quad + \sum_{k \in \mathbf{u}} \psi_k(\mathbf{x}) \sum_{\mathbf{v} \subseteq \mathbf{u} \setminus \{k\}} \nabla \partial_{\mathbf{v}}(u_h^{s_\ell} - u_h^{s_{\ell-1}}) \cdot \nabla \partial_{(\mathbf{u} \setminus \{k\}) \setminus \mathbf{v}} v_h^g. \end{aligned}$$

Thus

$$\begin{aligned} \left| \int_D \tilde{r}_{\mathbf{u}}(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} \right| &\leq a_{\max} \sum_{\mathbf{v} \subseteq \mathbf{u}} \|\partial_{\mathbf{v}}(u_h^{s_\ell} - u_h^{s_{\ell-1}})\|_V \|\partial_{\mathbf{u} \setminus \mathbf{v}} v_h^g\|_V \\ &\quad + \sum_{k \in \mathbf{u}} \|\psi_k\|_{L^\infty(D)} \sum_{\mathbf{v} \subseteq \mathbf{u} \setminus \{k\}} \|\partial_{\mathbf{v}}(u_h^{s_\ell} - u_h^{s_{\ell-1}})\|_V \|\partial_{(\mathbf{u} \setminus \{k\}) \setminus \mathbf{v}} v_h^g\|_V. \end{aligned} \quad (53)$$

For any  $\mathbf{y} \in U$ ,  $u_h^{s_\ell}(\cdot, \mathbf{y})$  and  $u_h^{s_{\ell-1}}(\cdot, \mathbf{y})$  are the solutions of the variational problems:

$$\begin{aligned} (a^{s_\ell}(\cdot, \mathbf{y}) \nabla u_h^{s_\ell}(\cdot, \mathbf{y}), \nabla v) &= (f, v) \quad \forall v \in V_h, \\ (a^{s_{\ell-1}}(\cdot, \mathbf{y}) \nabla u_h^{s_{\ell-1}}(\cdot, \mathbf{y}), \nabla v) &= (f, v) \quad \forall v \in V_h. \end{aligned}$$

Subtracting, we get  $(a^{s_\ell}(\cdot, \mathbf{y}) \nabla u_h^{s_\ell}(\cdot, \mathbf{y}) - a^{s_{\ell-1}}(\cdot, \mathbf{y}) \nabla u_h^{s_{\ell-1}}(\cdot, \mathbf{y}), \nabla v) = 0$  for all  $v \in V_h$ , or equivalently,

$$\begin{aligned} (a^{s_\ell}(\cdot, \mathbf{y}) \nabla(u_h^{s_\ell}(\cdot, \mathbf{y}) - u_h^{s_{\ell-1}}(\cdot, \mathbf{y})), \nabla v) \\ = -((a^{s_\ell}(\cdot, \mathbf{y}) - a^{s_{\ell-1}}(\cdot, \mathbf{y})) \nabla u_h^{s_{\ell-1}}(\cdot, \mathbf{y}), \nabla v) \quad \forall v \in V_h. \end{aligned}$$

We interpret this as a weak problem for  $u_h^{s_\ell}(\cdot, \mathbf{y}) - u_h^{s_{\ell-1}}(\cdot, \mathbf{y})$ , with the forcing term

$$\tilde{f} := \nabla \cdot ((a^{s_\ell}(\cdot, \mathbf{y}) - a^{s_{\ell-1}}(\cdot, \mathbf{y})) \nabla u_h^{s_{\ell-1}}(\cdot, \mathbf{y})) \in V^*.$$

Hence we conclude from (33) of Theorem 6, adapted to the finite element solutions, that

$$\|\partial_{\mathbf{v}}(u_h^{s_\ell} - u_h^{s_{\ell-1}})\|_V \leq |\mathbf{v}|! \left( \prod_{j \in \mathbf{v}} b_j \right) \frac{\|\tilde{f}\|_{V^*}}{a_{\min}}.$$

For any  $v \in V$ , we obtain with integration by parts and the Cauchy-Schwarz inequality, and Theorem 3

$$\begin{aligned} |(\tilde{f}, v)| &= \left| \int_D \nabla \cdot ((a^{s_\ell}(\mathbf{x}, \mathbf{y}) - a^{s_{\ell-1}}(\mathbf{x}, \mathbf{y})) \nabla u_h^{s_{\ell-1}}(\mathbf{x}, \mathbf{y})) v(\mathbf{x}) \, d\mathbf{x} \right| \\ &= \left| \int_D (a^{s_\ell}(\mathbf{x}, \mathbf{y}) - a^{s_{\ell-1}}(\mathbf{x}, \mathbf{y})) \nabla u_h^{s_{\ell-1}}(\mathbf{x}, \mathbf{y}) \cdot \nabla v(\mathbf{x}) \, d\mathbf{x} \right| \\ &\leq \left( \frac{1}{2} \sum_{j=s_{\ell-1}+1}^{s_\ell} \|\psi_j\|_{L^\infty(D)} \right) \|u_h^{s_{\ell-1}}(\cdot, \mathbf{y})\|_V \|v\|_V \\ &\leq \left( \frac{a_{\min}}{2} \sum_{j=s_{\ell-1}+1}^{s_\ell} b_j \right) \frac{\|f\|_{V^*}}{a_{\min}} \|v\|_V = \left( \frac{1}{2} \sum_{j=s_{\ell-1}+1}^{s_\ell} b_j \right) \|f\|_{V^*} \|v\|_V, \end{aligned}$$

which yields a bound on  $\|\tilde{f}\|_{V^*}$ , and in turn this gives

$$\|\partial_{\mathbf{v}}(u_h^{s_\ell} - u_h^{s_{\ell-1}})\|_V \leq |\mathbf{v}|! \left( \prod_{j \in \mathbf{v}} b_j \right) \left( \frac{1}{2} \sum_{j=s_{\ell-1}+1}^{s_\ell} b_j \right) \frac{\|f\|_{V^*}}{a_{\min}}. \quad (54)$$

Next, from (47) we can interpret  $v_h^g$  as the solution of the weak problem (9) with the forcing term  $g$ . Thus we can apply (33) of Theorem 6 again to obtain

$$\|\partial_{\mathbf{u} \setminus \mathbf{v}} v_h^g\|_V \leq |\mathbf{u} \setminus \mathbf{v}|! \left( \prod_{j \in \mathbf{u} \setminus \mathbf{v}} b_j \right) \frac{\|g\|_{V^*}}{a_{\min}} = |\mathbf{u} \setminus \mathbf{v}|! \left( \prod_{j \in \mathbf{u} \setminus \mathbf{v}} b_j \right) \frac{\|G(\cdot)\|_{V^*}}{a_{\min}}. \quad (55)$$

Using (54), (55), and again  $\sum_{\mathbf{v} \subseteq \mathbf{u}} |\mathbf{v}|! |\mathbf{u} \setminus \mathbf{v}|! = (|\mathbf{u}| + 1)!$ , we obtain from (53)

$$\begin{aligned} &\left| \int_D \tilde{r}_{\mathbf{u}}(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} \right| \\ &\leq \left( \frac{1}{2} \sum_{j=s_{\ell-1}+1}^{s_\ell} b_j \right) \frac{\|f\|_{V^*} \|G(\cdot)\|_{V^*}}{a_{\min}^2} \left[ a_{\max} \sum_{\mathbf{v} \subseteq \mathbf{u}} |\mathbf{v}|! \left( \prod_{j \in \mathbf{v}} b_j \right) |\mathbf{u} \setminus \mathbf{v}|! \left( \prod_{j \in \mathbf{u} \setminus \mathbf{v}} b_j \right) \right. \\ &\quad \left. + a_{\min} \sum_{k \in \mathbf{u}} b_k \sum_{\mathbf{v} \subseteq \mathbf{u} \setminus \{k\}} |\mathbf{v}|! \left( \prod_{j \in \mathbf{v}} b_j \right) |(\mathbf{u} \setminus \{k\}) \setminus \mathbf{v}|! \left( \prod_{j \in (\mathbf{u} \setminus \{k\}) \setminus \mathbf{v}} b_j \right) \right] \\ &= \left( \frac{1}{2} \sum_{j=s_{\ell-1}+1}^{s_\ell} b_j \right) \left( \prod_{j \in \mathbf{u}} b_j \right) \frac{\|f\|_{V^*} \|G(\cdot)\|_{V^*}}{a_{\min}^2} \left[ a_{\max} (|\mathbf{u}| + 1)! + a_{\min} |\mathbf{u}|! \right] \\ &\leq \left( \sum_{j=s_{\ell-1}+1}^{s_\ell} b_j \right) \left( \prod_{j \in \mathbf{u}} b_j \right) \frac{\|f\|_{V^*} \|G(\cdot)\|_{V^*}}{a_{\min}^2} a_{\max} (|\mathbf{u}| + 1)!. \end{aligned}$$

Substituting this estimate into (52) completes the proof.  $\square$

### 3.5 Error Analysis of the Multi-level QMC-FE Algorithm (Continued)

We are now ready to estimate the two terms in (26) for  $\ell \neq 0$ . To bound the first term, we use the triangle inequality

$$\|G(u_{h_\ell}^{s_\ell} - u_{h_{\ell-1}}^{s_\ell})\|_{\mathcal{H}_{s_\ell, \boldsymbol{\gamma}}} \leq \|G(u^{s_\ell} - u_{h_\ell}^{s_\ell})\|_{\mathcal{H}_{s_\ell, \boldsymbol{\gamma}}} + \|G(u^{s_\ell} - u_{h_{\ell-1}}^{s_\ell})\|_{\mathcal{H}_{s_\ell, \boldsymbol{\gamma}}},$$

and then apply Theorem 7 to both terms on the right-hand side. If  $k$ -orthogonality (28) does not hold and if  $s_\ell \neq s_{\ell-1}$ , we bound the second term in (26) using Theorem 8. For the  $\ell = 0$  term in (25), we use the estimate

$$\begin{aligned} \|G(u_{h_0}^{s_0})\|_{\mathcal{H}_{s_0, \boldsymbol{\gamma}}} &\leq \left( \sum_{\mathbf{u} \subseteq \{1:s_0\}} \frac{1}{\gamma_{\mathbf{u}}} \int_{[-\frac{1}{2}, \frac{1}{2}]^{|\mathbf{u}|}} \|G(\cdot)\|_{V^*}^2 \left\| \frac{\partial^{|\mathbf{u}|} u_{h_0}(\cdot, (\mathbf{y}_{\mathbf{u}}; 0))}{\partial \mathbf{y}_{\mathbf{u}}} \right\|_V^2 d\mathbf{y}_{\mathbf{u}} \right)^{1/2} \\ &\leq \frac{\|f\|_{V^*} \|G(\cdot)\|_{V^*}}{a_{\min}} \left( \sum_{\mathbf{u} \subseteq \{1:s_0\}} \frac{(|\mathbf{u}|!)^2 \prod_{j \in \mathbf{u}} b_j^2}{\gamma_{\mathbf{u}}} \right)^{1/2}, \end{aligned}$$

which follows from an adaptation of (33) from Theorem 6. Combining these estimates with (22), (24), (25), and (26), we obtain

$$\begin{aligned} &\mathbb{E}[|I(G(u)) - Q_*^L(\cdot; G(u))|^2] \\ &\leq C \left( \left[ h_L^\tau \|f\|_{H^{-1+t}(D)} \|G(\cdot)\|_{H^{-1+t'}(D)} + \theta_L \|f\|_{V^*} \|G(\cdot)\|_{V^*} \left( \sum_{j \geq s_L+1} b_j \right)^2 \right]^2 \right. \\ &\quad + \left( \sum_{\emptyset \neq \mathbf{u} \subseteq \{1:s_0\}} \gamma_{\mathbf{u}}^\lambda [\rho(\lambda)]^{|\mathbf{u}|} \right)^{1/\lambda} [\varphi(N_0)]^{-1/\lambda} \|f\|_{V^*}^2 \|G(\cdot)\|_{V^*}^2 \sum_{\mathbf{u} \subseteq \{1:s_0\}} \frac{(|\mathbf{u}|!)^2 \prod_{j \in \mathbf{u}} b_j^2}{\gamma_{\mathbf{u}}} \\ &\quad + \sum_{\ell=1}^L \left( \sum_{\emptyset \neq \mathbf{u} \subseteq \{1:s_\ell\}} \gamma_{\mathbf{u}}^\lambda [\rho(\lambda)]^{|\mathbf{u}|} \right)^{1/\lambda} [\varphi(N_\ell)]^{-1/\lambda} \\ &\quad \cdot \left[ h_{\ell-1}^\tau \|f\|_{H^{-1+t}(D)} \|G(\cdot)\|_{H^{-1+t'}(D)} \left( \sum_{\mathbf{u} \subseteq \{1:s_\ell\}} \frac{[(|\mathbf{u}|+1)!]^2 \prod_{j \in \mathbf{u}} \bar{b}_j^2}{\gamma_{\mathbf{u}}} \right)^{1/2} \right. \\ &\quad \left. + \theta_{\ell-1} \|f\|_{V^*} \|G(\cdot)\|_{V^*} \left( \sum_{j=s_{\ell-1}+1}^{s_\ell} b_j \right) \left( \sum_{\mathbf{u} \subseteq \{1:s_\ell\}} \frac{[(|\mathbf{u}|+1)!]^2 \prod_{j \in \mathbf{u}} b_j^2}{\gamma_{\mathbf{u}}} \right)^{1/2} \right]^2 \Big), \end{aligned}$$

where we introduced the parameters  $\theta_{\ell-1} \in \{0, 1\}$  for each level, analogously to (24), to handle the case where  $k$ -orthogonality (28) holds or when  $s_\ell = s_{\ell-1}$ .

When  $k$ -orthogonality (28) does not hold, we further impose Assumptions **(A3)** and **(A5)** to make use of (14) for estimating the tail sums of  $b_j$ . These together with some further estimations lead to the following simplified mean-square error bound.

**Theorem 9** *Under Assumptions **(A1)**–**(A6)**, for every  $f \in H^{-1+t}(D)$  with  $0 \leq t \leq 1$  and every  $G(\cdot) \in H^{-1+t'}(D)$  with  $0 \leq t' \leq 1$ , the mean-square error of the multi-level*

QMC-FE algorithm defined by (19) can be estimated as follows

$$\mathbb{E}[|I(G(u)) - Q_*^L(\cdot; G(u))|^2] \leq CD_{\boldsymbol{\gamma}}(\lambda) \|f\|_{H^{-1+t}(D)}^2 \|G(\cdot)\|_{H^{-1+t'}(D)}^2 \cdot \left[ \left( h_L^\tau + \theta_L s_L^{-2(1/p-1)} \right)^2 + \sum_{\ell=0}^L [\varphi(N_\ell)]^{-1/\lambda} \left( h_{\ell-1}^\tau + \theta_{\ell-1} s_{\ell-1}^{-2(1/p-1)} \right)^2 \right], \quad (56)$$

where

$$D_{\boldsymbol{\gamma}}(\lambda) := \left( \sum_{|\mathbf{u}| < \infty} \gamma_{\mathbf{u}}^\lambda [\rho(\lambda)]^{|\mathbf{u}|} \right)^{1/\lambda} \left( \sum_{|\mathbf{u}| < \infty} \frac{[(|\mathbf{u}|+1)!]^2 \prod_{j \in \mathbf{u}} \bar{b}_j^2}{\gamma_{\mathbf{u}}} \right), \quad (57)$$

with  $0 \leq \tau := t + t' \leq 2$ ,  $h_{-1} \equiv \theta_{-1} \equiv s_{-1} \equiv 0$ ,  $\rho(\lambda)$  as in (17), and  $\bar{b}_j$  as in (35). In general we have  $\theta_\ell = 1$  for all  $\ell = 0, \dots, L$ . If  $s_\ell = s_{\ell-1}$  for some  $\ell \geq 1$  then  $\theta_{\ell-1} = 0$ . When  $k$ -orthogonality (28) holds we have  $\theta_\ell = 0$  for all  $\ell = 0, \dots, L$ . Assumptions (A3) and (A5) are not required when  $\theta_\ell = 0$  for all  $\ell$ . The expectation  $\mathbb{E}[\cdot]$  is with respect to the random compound shift which is drawn from the uniform distribution over  $[0, 1]^{s^*}$ . The error bound (56) is meaningful only if  $D_{\boldsymbol{\gamma}}(\lambda)$  is finite.

### 3.6 Choosing the Parameter $\lambda$ and the Weights $\gamma_{\mathbf{u}}$

Following [23], we now choose the weights  $\gamma_{\mathbf{u}}$  to minimize  $D_{\boldsymbol{\gamma}}(\lambda)$ . We also specify the value of  $\lambda$  to get the best convergence rate possible. Note that our goal is to have  $\lambda$  as small as possible, since a smaller value of  $\lambda$  yields a better convergence rate with respect to the number of QMC points. In the following theorem, the assumption (58) is implied by Assumption (A7).

**Theorem 10** With  $\bar{b}_j$  defined as in (35) for fixed  $\kappa \in (0, 1]$ , suppose that

$$\sum_{j \geq 1} \bar{b}_j^q < \infty \quad \text{for some } 0 < q \leq 1, \quad (58)$$

and when  $q = 1$  assume additionally that

$$\sum_{j \geq 1} \bar{b}_j < 2. \quad (59)$$

For a given  $\lambda \in (1/2, 1]$ , the choice of weights

$$\gamma_{\mathbf{u}} = \gamma_{\mathbf{u}}^*(\lambda) := \left( (|\mathbf{u}|+1)! \prod_{j \in \mathbf{u}} \frac{\bar{b}_j}{\sqrt{\rho(\lambda)}} \right)^{2/(1+\lambda)} \quad (60)$$

minimizes  $D_{\boldsymbol{\gamma}}(\lambda)$  given in (57), if a finite minimum exists. Moreover, the choice of  $\lambda$  given by

$$\lambda = \lambda_q := \begin{cases} \frac{1}{2-2\delta} & \text{for some } \delta \in (0, 1/2) \quad \text{when } q \in (0, 2/3], \\ \frac{q}{2-q} & \text{when } q \in (2/3, 1), \\ 1 & \text{when } q = 1, \end{cases} \quad (61)$$



together with  $\gamma_{\mathbf{u}} = \gamma_{\mathbf{u}}^*(\lambda_q)$ , ensures that  $D_{\boldsymbol{\gamma}}(\lambda) < \infty$ , and thus justifies the error bound (56).

If we maintain the definition (61) of  $\lambda$  but instead of (60) define the weights by

$$\gamma_{\mathbf{u}} := \left( (|\mathbf{u}| + 1)! \prod_{j \in \mathbf{u}} (2\bar{b}_j) \right)^{2-q}, \quad (62)$$

then  $D_{\boldsymbol{\gamma}}(\lambda)$  is no longer minimized by this choice of weights, but  $D_{\boldsymbol{\gamma}}(\lambda) < \infty$  still holds provided that  $\delta < q/2$  when  $q \in (0, 2/3]$ .

We remark that the weight (62) has a practical advantage over (60), that with (62) it is not necessary to make a prior choice of  $\lambda$ .

*Proof* This proof follows closely the proofs of [23, Theorems 6.4 and 6.5]. Apart from the simple replacement of  $b_j$  by  $\bar{b}_j$  and of  $p$  by  $q$ , the main difference is that we now have to handle a sum containing the factor  $(|\mathbf{u}| + 1)!$  instead of  $|\mathbf{u}|!$ . For this we make use of [23, Lemma 6.3] with  $n = 1$  instead of  $n = 0$ .

Using [23, Lemma 6.2], we see that  $D_{\boldsymbol{\gamma}}(\lambda)$  is minimized by choosing  $\gamma_{\mathbf{u}}$  as in (60) for  $|\mathbf{u}| < \infty$ , provided that a finite minimum exists. The relative scaling of weights does not affect the minimization argument. Our choice of scaling here is consistent with the convention that  $\gamma_{\emptyset} = 1$ .

In the course of our derivation below we eventually choose the value of  $\lambda$  depending on the value of  $q$ , but until then  $\lambda$  and  $q$  will be independent. For the weights given by (60), we have

$$\begin{aligned} \sum_{|\mathbf{u}| < \infty} (\gamma_{\mathbf{u}}^*)^\lambda [\rho(\lambda)]^{|\mathbf{u}|} &= \sum_{|\mathbf{u}| < \infty} [(|\mathbf{u}| + 1)!]^{2\lambda/(1+\lambda)} \prod_{j \in \mathbf{u}} \left( \bar{b}_j^{2\lambda} \rho(\lambda) \right)^{1/(1+\lambda)} =: A_\lambda, \\ \sum_{|\mathbf{u}| < \infty} \frac{[ (|\mathbf{u}| + 1)! ]^2 \prod_{j \in \mathbf{u}} \bar{b}_j^2}{\gamma_{\mathbf{u}}^*} &= A_\lambda, \end{aligned}$$

and thus  $D_{\boldsymbol{\gamma}^*}(\lambda) = A_\lambda^{1/\lambda+1}$ .

For  $\lambda \in (1/2, 1)$ , we have  $2\lambda/(1+\lambda) < 1$  and we further estimate  $A_\lambda$  as follows: we multiply and divide each term in the expression by  $\prod_{j \in \mathbf{u}} \alpha_j^{2\lambda/(1+\lambda)}$ , with  $\alpha_j > 0$  to be specified later, and then apply Hölder's inequality with conjugate exponents  $(1+\lambda)/(2\lambda)$  and  $(1+\lambda)/(1-\lambda)$ , to obtain

$$\begin{aligned} A_\lambda &= \sum_{|\mathbf{u}| < \infty} [ (|\mathbf{u}| + 1)! ]^{2\lambda/(1+\lambda)} \prod_{j \in \mathbf{u}} \alpha_j^{2\lambda/(1+\lambda)} \prod_{j \in \mathbf{u}} \left( \frac{\bar{b}_j^{2\lambda} \rho(\lambda)}{\alpha_j^{2\lambda}} \right)^{1/(1+\lambda)} \\ &\leq \left( \sum_{|\mathbf{u}| < \infty} (|\mathbf{u}| + 1)! \prod_{j \in \mathbf{u}} \alpha_j \right)^{2\lambda/(1+\lambda)} \left( \sum_{|\mathbf{u}| < \infty} \prod_{j \in \mathbf{u}} \left( \frac{\bar{b}_j^{2\lambda} \rho(\lambda)}{\alpha_j^{2\lambda}} \right)^{1/(1-\lambda)} \right)^{(1-\lambda)/(1+\lambda)} \\ &\leq \left( \frac{1}{1 - \sum_{j \geq 1} \alpha_j} \right)^{4\lambda/(1+\lambda)} \exp \left( \frac{1-\lambda}{1+\lambda} [\rho(\lambda)]^{1/(1-\lambda)} \sum_{j \geq 1} \left( \frac{\bar{b}_j}{\alpha_j} \right)^{2\lambda/(1-\lambda)} \right) \end{aligned}$$

which holds and  $A_\lambda$  is finite, see [23, Lemma 6.3], provided that

$$\sum_{j \geq 1} \alpha_j < 1 \quad \text{and} \quad \sum_{j \geq 1} \left( \frac{\bar{b}_j}{\alpha_j} \right)^{2\lambda/(1-\lambda)} < \infty. \quad (63)$$

We now choose

$$\alpha_j := \frac{\bar{b}_j^q}{\varpi} \quad \text{for some parameter } \varpi > \sum_{j \geq 1} \bar{b}_j^q. \quad (64)$$

Then the first sum in (63) is less than 1 due to the assumption (58). Noting that (58) implies that  $\sum_{j \geq 1} \bar{b}_j^{q'} < \infty$  for all  $q' \geq q$ , we conclude that the second sum in (63) converges for

$$\frac{2\lambda}{1-\lambda}(1-q) \geq q \quad \iff \quad q \leq \frac{2\lambda}{1+\lambda} \quad \iff \quad \lambda \geq \frac{q}{2-q}.$$

Since  $\lambda$  must be strictly between  $1/2$  and  $1$ , when  $q \in (0, 2/3]$  we choose  $\lambda_q = 1/(2 - 2\delta)$  for some  $\delta \in (0, 1/2)$ , and when  $q \in (2/3, 1)$  we set  $\lambda_q = q/(2 - q)$ .

For the case  $q = 1$  we take  $\lambda_q = 1$ , and we use  $\rho(1) = 1/4$ . Then using [23, Lemma 6.3] and the assumption (59) we obtain

$$A_1 = \sum_{|u| < \infty} (|u| + 1)! \prod_{j \in u} \left( \frac{\bar{b}_j}{2} \right) \leq \left( \frac{1}{1 - \sum_{j \geq 1} (\bar{b}_j/2)} \right)^2 < \infty.$$

Finally we show that  $D_{\mathcal{Y}}(\lambda) < \infty$  for  $\lambda$  given by (61) and weights given by (62). For the case  $q = 1$  and  $\lambda = 1$ , the weights (60) and (62) are the same, so we need to consider only the cases  $q \in (0, 2/3]$  and  $q \in (2/3, 1)$ . To simplify the presentation below we introduce  $q' := \lambda(2 - q)$ . Then, with  $\lambda$  given by (61), with the additional restriction that  $\delta < q/2$ , it is easy to verify that  $q' = q$  for  $q \in (2/3, 1)$  and  $q < q' < 1$  for  $q \in (0, 2/3]$ . In both cases, we have

$$D_{\mathcal{Y}}(\lambda) = \left( \sum_{|u| < \infty} [(|u| + 1)!]^{q'} \prod_{j \in u} \left( (2\bar{b}_j)^{q'} \rho(\lambda) \right) \right)^{\frac{2-q}{q'}} \left( \sum_{|u| < \infty} [(|u| + 1)!]^q \prod_{j \in u} \frac{\bar{b}_j^q}{2^{2-q}} \right).$$

For the first sum, we multiply and divide the terms by  $\prod_{j \in u} \alpha_j^{q'}$ , with  $\alpha_j > 0$  to be specified later, and we apply Hölder's inequality with conjugate exponents  $1/q'$  and  $1/(1 - q')$ . For the second sum, we multiply and divide the terms by  $\prod_{j \in u} \alpha_j^q$ , with the same  $\alpha_j$ , and we apply Hölder's inequality with conjugate exponents  $1/q$  and  $1/(1 - q)$ . We obtain

$$\begin{aligned} D_{\mathcal{Y}}(\lambda) &\leq \left( \sum_{|u| < \infty} (|u| + 1)! \prod_{j \in u} \alpha_j \right)^{2-q} \left( \sum_{|u| < \infty} \prod_{j \in u} \left( \frac{(2\bar{b}_j)^{q'} \rho(\lambda)}{\alpha_j^{q'}} \right)^{\frac{1}{1-q'}} \right)^{\frac{(1-q')(2-q)}{q'}} \\ &\quad \times \left( \sum_{|u| < \infty} (|u| + 1)! \prod_{j \in u} \alpha_j \right)^q \left( \sum_{|u| < \infty} \prod_{j \in u} \left( \frac{\bar{b}_j^q}{2^{2-q} \alpha_j^q} \right)^{\frac{1}{1-q}} \right)^{1-q}, \end{aligned}$$

which is finite as above provided that

$$\sum_{j \geq 1} \alpha_j < 1, \quad \sum_{j \geq 1} \left( \frac{\bar{b}_j}{\alpha_j} \right)^{\frac{q'}{1-q'}} < \infty, \quad \text{and} \quad \sum_{j \geq 1} \left( \frac{\bar{b}_j}{\alpha_j} \right)^{\frac{q}{1-q}} < \infty,$$

and this can be achieved by choosing  $\alpha_j$  as in (64), since  $q'/(1-q') \geq q/(1-q)$ . This completes the proof.  $\square$

### 3.7 Summary of Overall Cost Versus Error

Recall that

$$h_\ell \asymp 2^{-\ell} \quad \text{and} \quad M_{h_\ell} \asymp h_\ell^{-d} \asymp 2^{\ell d} \quad \text{for} \quad \ell = 0, \dots, L. \quad (65)$$

Based on the mean square error bound (56), we now specify  $s_\ell$  and  $N_\ell$  for each level. We consider two scenarios depending on whether or not  $k$ -orthogonality (28) holds.

For our cost model we assume the availability of a linear complexity FE solver. The cost for assembling the stiffness matrix at level  $\ell$  is  $\mathcal{O}(s_\ell M_{h_\ell})$  in general, and is  $\mathcal{O}(M_{h_\ell} \log(M_{h_\ell}))$  if  $k$ -orthogonality (28) holds (see the second part of Theorem 5). Moreover, we assume that the functions  $\psi_j$  are explicitly known, and that integration of any basis functions in the FE method against any  $\psi_j$  is available at unit cost. Thus

$$\text{cost} = \mathcal{O} \left( \sum_{\ell=0}^L N_\ell K_\ell \right), \quad K_\ell := \begin{cases} h_\ell^{-d} \log(h_\ell^{-d}) & \text{if } k\text{-orthogonality (28) holds,} \\ h_\ell^{-d} s_\ell & \text{otherwise.} \end{cases}$$

Clearly, changing the cost model may change the definition of  $K_\ell$ . (Some cost models in the literature do not include  $s_\ell$  as part of  $K_\ell$ .) Note that our cost model does not include the pre-computation cost for the CBC construction of randomly shifted lattice rules, which requires  $\mathcal{O}(N_\ell \log N_\ell s_\ell + N_\ell s_\ell^2)$  operations on level  $\ell$ .

*Scenario 1.* In the special case where  $k$ -orthogonality (28) holds, the values of  $s_\ell$  are given by (29), and we have  $\theta_\ell = 0$  for all  $\ell$  in the error bound (56), giving the mean square error bound (denoted in this subsection by  $\text{error}^2$  for simplicity)

$$\text{error}^2 = \mathcal{O} \left( h_L^{2\tau} + \sum_{\ell=0}^L [\varphi(N_\ell)]^{-1/\lambda} h_{\ell-1}^{2\tau} \right). \quad (66)$$

*Scenario 2.* When  $k$ -orthogonality (28) does not hold, we have  $\theta_L = 1$  in the error bound (56). To balance the error contribution within the highest discretization level, we impose the condition  $s_L^{-2(1/p-1)} = \mathcal{O}(h_L^\tau)$ , which is equivalent to  $s_L = \Omega(2^{L\tau p/(2-2p)})$ . Then, to minimize the error within each level, one choice for  $s_\ell$  is to set  $s_\ell = s_L$  for all  $\ell < L$ , leading to  $\theta_{\ell-1} = 0$  for all  $\ell = 1, \dots, L$  in (56). Alternatively, since  $s_\ell$  should be as small as possible from the point of view of reducing the cost at each level, we can impose the condition  $s_{\ell-1}^{-2(1/p-1)} = \mathcal{O}(h_{\ell-1}^\tau)$  for  $\ell = 1, \dots, L$ , which

is equivalent to  $s_\ell = \Omega(2^{\ell\tau p/(1-p)})$  for  $\ell = 0, \dots, L-1$ . Combining both approaches, while taking into account the monotonicity condition (18), we choose

$$s_\ell := \min \left( \lceil 2^{\ell\tau p/(1-p)} \rceil, \lceil 2^{L\tau p/(2-2p)} \rceil \right) \quad \text{for } \ell = 0, \dots, L. \quad (67)$$

Thus we have  $s_\ell$  strictly increasing for  $\ell = 0, \dots, \lfloor L/2 \rfloor$ , and the remaining half of  $s_\ell$  are all identical. Our choice of  $s_\ell$  leads again to the error bound (66).

We remark that for all  $N \in \mathbb{N}$ , the Euler totient function  $\varphi(N)$  takes values close to  $N$ . Specifically, if  $N$  is prime then  $1/\varphi(N) = 1/(N-1) \leq 2/N$ . If  $N$  is a power of 2 then  $1/\varphi(N) = 2/N$ . It is known from [1, Theorem 8.8.7] that  $1/\varphi(N) < (e^\gamma \log \log N + 3/\log \log N)/N$  for all  $N \geq 3$ , where  $e^\gamma = 1.781\dots$ . Thus it can be verified that for all computationally realistic values of  $N$ , say,  $N \leq 10^{30}$ , we have  $1/\varphi(N) < 9/N$ . Treating this factor 9 as a constant and using  $h_{\ell-1} \asymp h_\ell$ , we obtain for both scenarios the simpler mean square error expression

$$\text{error}^2 = \mathcal{O} \left( h_L^{2\tau} + \sum_{\ell=0}^L N_\ell^{-1/\lambda} h_\ell^{2\tau} \right).$$

To minimize the mean square error for a fixed cost, we consider the Lagrange multiplier function

$$g(\mu) := \underbrace{h_L^{2\tau} + \sum_{\ell=0}^L N_\ell^{-1/\lambda} h_\ell^{2\tau}}_{\text{mean square error}} + \mu \underbrace{\sum_{\ell=0}^L N_\ell K_\ell}_{\text{cost}}.$$

We look for the stationary point of  $g(\mu)$  with respect to  $N_\ell$ , thus demanding that

$$\frac{\partial g(\mu)}{\partial N_\ell} = -\frac{1}{\lambda} N_\ell^{-1/\lambda-1} h_\ell^{2\tau} + \mu K_\ell = 0 \quad \text{for } \ell = 0, \dots, L.$$

This prompts us to define

$$N_\ell := \left[ N_0 (h_0^{-2\tau} K_0 h_\ell^{2\tau} K_\ell^{-1})^{\lambda/(\lambda+1)} \right] \quad \text{for } \ell = 1, \dots, L. \quad (68)$$

Leaving  $N_0$  to be specified later and treating  $h_0$  and  $K_0$  as constants, we conclude that

$$\text{error}^2 = \mathcal{O} \left( h_L^{2\tau} + N_0^{-1/\lambda} \sum_{\ell=0}^L E_\ell \right) \quad \text{and} \quad \text{cost} = \mathcal{O} \left( N_0 \sum_{\ell=0}^L E_\ell \right), \quad (69)$$

where

$$E_\ell := (h_\ell^{2\lambda\tau} K_\ell)^{1/(\lambda+1)} = \begin{cases} (h_\ell^{2\lambda\tau-d} \log(h_\ell^{-d}))^{1/(\lambda+1)} & \text{if } k\text{-orthogonality (28) holds,} \\ (h_\ell^{2\lambda\tau-d} s_\ell)^{1/(\lambda+1)} & \text{otherwise.} \end{cases}$$

We see that the mean square error is *not* necessarily minimized by balancing the error terms between the levels. For example, when  $k$ -orthogonality (28) holds, we observe that

- For  $d > 2\lambda\tau$ , the quantity  $E_\ell$  (and thus the mean square error and cost at level  $\ell$ ) increases with increasing  $\ell$ .
- For  $d < 2\lambda\tau$ , the quantity  $E_\ell$  decreases with increasing  $\ell$ .

*Scenario 1 (continued).* Substituting  $h_\ell \asymp 2^{-\ell}$ , we obtain for the case where  $k$ -orthogonality holds that

$$\begin{aligned} \sum_{\ell=0}^L E_\ell &= \mathcal{O} \left( \sum_{\ell=0}^L 2^{-\ell(2\lambda\tau-d)/(\lambda+1)} (\ell+1)^{1/(\lambda+1)} \right) \\ &= \begin{cases} \mathcal{O}(1) & \text{if } d < 2\lambda\tau, \\ \mathcal{O}(L^{(\lambda+2)/(\lambda+1)}) & \text{if } d = 2\lambda\tau, \\ \mathcal{O}(2^{-L(2\lambda\tau-d)/(\lambda+1)} L^{1/(\lambda+1)}) & \text{if } d > 2\lambda\tau. \end{cases} \end{aligned}$$

In light of the error bound in (69), we choose  $N_0$  to satisfy

$$N_0^{-1/\lambda} \sum_{\ell=0}^L E_\ell = \mathcal{O}(h_L^{2\tau}), \quad (70)$$

which is equivalent to  $N_0 = \Omega(h_L^{-2\tau\lambda} (\sum_{\ell=0}^L E_\ell)^\lambda)$ . This yields the choice

$$N_0 := \begin{cases} \lceil 2^{L\tau(2\lambda)} \rceil & \text{if } d < 2\tau\lambda, \\ \lceil 2^{L\tau(2\lambda)} L^{\lambda(\lambda+2)/(\lambda+1)} \rceil & \text{if } d = 2\tau\lambda, \\ \lceil 2^{L\tau(d/\tau+2)\lambda/(\lambda+1)} L^{\lambda/(\lambda+1)} \rceil & \text{if } d > 2\tau\lambda. \end{cases} \quad (71)$$

Then we have  $\text{error}^2 = \mathcal{O}(h_L^{2\tau})$ . Upon substituting (70) into the cost bound in (69) and using (71), we obtain

$$\text{cost} = \mathcal{O}(N_0^{(\lambda+1)/\lambda} h_L^{2\tau}) = \begin{cases} \mathcal{O}(2^{L\tau(2\lambda)}) & \text{if } d < 2\lambda\tau, \\ \mathcal{O}(2^{L\tau(2\lambda)} L^{\lambda+2}) & \text{if } d = 2\lambda\tau, \\ \mathcal{O}(2^{L\tau(d/\tau)} L) & \text{if } d > 2\lambda\tau. \end{cases}$$

*Scenario 2 (continued).* When  $k$ -orthogonality does not hold, we use the definition (67) for  $s_\ell$  and denote for simplicity

$$\alpha := \frac{p}{1-p},$$

to obtain

$$\begin{aligned} \sum_{\ell=0}^L E_\ell &= \mathcal{O} \left( \sum_{\ell=0}^{\lfloor L/2 \rfloor} 2^{-\ell\tau(2\lambda-d/\tau-\alpha)/(\lambda+1)} + 2^{(L/2)\tau\alpha/(\lambda+1)} \sum_{\ell=\lfloor L/2 \rfloor+1}^L 2^{-\ell\tau(2\lambda-d/\tau)/(\lambda+1)} \right) \\ &= \begin{cases} \mathcal{O}(1) & \text{if } d/\tau < 2\lambda - \alpha, \\ \mathcal{O}(L) & \text{if } d/\tau = 2\lambda - \alpha, \\ \mathcal{O}(2^{L\tau(\alpha/2+d/(2\tau)-\lambda)/(\lambda+1)}) & \text{if } 2\lambda - \alpha < d/\tau < 2\lambda, \\ \mathcal{O}(2^{L\tau(\alpha/2)/(\lambda+1)} L) & \text{if } d/\tau = 2\lambda, \\ \mathcal{O}(2^{L\tau(\alpha/2+d/\tau-2\lambda)/(\lambda+1)}) & \text{if } d/\tau > 2\lambda. \end{cases} \end{aligned}$$

As in Scenario 1 we choose  $N_0$  to satisfy (70), i.e.,  $N_0 = \Omega(h_L^{-2\tau\lambda} (\sum_{\ell=0}^L E_\ell)^\lambda)$ , and this yields

$$N_0 := \begin{cases} \lceil 2^{L\tau(2\lambda)} \rceil & \text{if } d/\tau < 2\lambda - \alpha, \\ \lceil 2^{L\tau(2\lambda)} L^\lambda \rceil & \text{if } d/\tau = 2\lambda - \alpha, \\ \lceil 2^{L\tau(\alpha/2+d/(2\tau)+\lambda+2)\lambda/(\lambda+1)} \rceil & \text{if } 2\lambda - \alpha < d/\tau < 2\lambda, \\ \lceil 2^{L\tau(\alpha/2+d/\tau+2)\lambda/(\lambda+1)} L^\lambda \rceil & \text{if } d/\tau = 2\lambda, \\ \lceil 2^{L\tau(\alpha/2+d/\tau+2)\lambda/(\lambda+1)} \rceil & \text{if } d/\tau > 2\lambda. \end{cases} \quad (72)$$

Then we have  $\text{error}^2 = \mathcal{O}(h_L^{2\tau})$  as before, but now

$$\text{cost} = \mathcal{O}(N_0^{(\lambda+1)/\lambda} h_L^{2\tau}) = \begin{cases} \mathcal{O}(2^{L\tau(2\lambda)}) & \text{if } d/\tau < 2\lambda - \alpha, \\ \mathcal{O}(2^{L\tau(2\lambda)} L^{\lambda+1}) & \text{if } d/\tau = 2\lambda - \alpha, \\ \mathcal{O}(2^{L\tau(\alpha/2+d/(2\tau)+\lambda)}) & \text{if } 2\lambda - \alpha < d/\tau < 2\lambda, \\ \mathcal{O}(2^{L\tau(\alpha/2+d/\tau)} L^{\lambda+1}) & \text{if } d/\tau = 2\lambda, \\ \mathcal{O}(2^{L\tau(\alpha/2+d/\tau)}) & \text{if } d/\tau > 2\lambda. \end{cases}$$

In both scenarios, for given  $\varepsilon > 0$ , we choose  $L$  such that

$$h_L^\tau \asymp 2^{-L\tau} \asymp \varepsilon. \quad (73)$$

We can then express the total cost of the algorithm in terms of  $\varepsilon$ . This is summarized in Theorem 11 below.

**Theorem 11** *Under Assumptions (A1)–(A7), leaving out (A5) if  $k$ -orthogonality (28) holds, for  $f \in H^{-1+t}(D)$  and  $G(\cdot) \in H^{-1+t'}(D)$  with  $0 \leq t, t' \leq 1$  and  $\tau := t + t' > 0$ , we consider the multi-level QMC-FE algorithm defined by (19). Given  $\varepsilon > 0$ , with  $L$  given by (73),  $h_\ell$  given by (65),  $s_\ell$  given by (67) (or (29) under  $k$ -orthogonality),  $N_\ell$  given by (68),  $N_0$  given by (72) (or (71) under  $k$ -orthogonality), and with randomly shifted lattice rules constructed based on POD weights  $\gamma_u$  given by (60) or (62), we obtain*

$$\sqrt{\mathbb{E}[|I(G(u)) - Q_*^L(\cdot; G(u))|^2]} = \mathcal{O}(\varepsilon),$$

and

$$\text{cost}(Q_*^L) = \mathcal{O}(\varepsilon^{-a^{\text{ML}}} (\log \varepsilon^{-1})^{b^{\text{ML}}}),$$

with

$$a^{\text{ML}} = \begin{cases} \max\left(2\lambda_q, \frac{d}{\tau}\right) & \text{if } k\text{-orthogonality (28) holds,} \\ 2\lambda_q & \text{if } \frac{d}{\tau} \leq 2\lambda_q - \frac{p}{1-p}, \\ \frac{p}{2-2p} + \frac{d}{2\tau} + \max\left(\lambda_q, \frac{d}{2\tau}\right) & \text{if } \frac{d}{\tau} > 2\lambda_q - \frac{p}{1-p}, \end{cases}$$

where  $\lambda_q$  is as defined in (61). The value of  $b^{\text{ML}}$  can be obtained from the cost bounds in Scenarios 1 and 2 in a similar way.

In comparison, for the single level QMC-FE algorithm in [23] to achieve  $\mathcal{O}(\varepsilon)$  error, its overall cost in the case of  $p < 1$  is  $\mathcal{O}(\varepsilon^{-a^{\text{SL}}})$ , with

$$a^{\text{SL}} = \frac{p}{2-2p} + 2\lambda_p + \frac{d}{\tau},$$

see [23, Theorem 8.1], where  $\lambda_p$  is defined analogously to  $\lambda_q$  as follows

$$\lambda_p := \begin{cases} \frac{1}{2-p} & \text{for some } \delta \in (0, 1/2) \text{ when } p \in (0, 2/3], \\ \frac{p}{2-p} & \text{when } p \in (2/3, 1). \end{cases}$$

Note that  $a^{\text{ML}}$  is much smaller than  $a^{\text{SL}}$  in most cases. This is clearly seen when  $\lambda_q \approx \lambda_p$ . However, in the extreme case where  $\lambda_q$  and  $\lambda_p$  are furthest apart, i.e,  $\lambda_q = 1$  and  $\lambda_p \approx 1/2$ , it is possible to come up with an example where  $a^{\text{SL}} < a^{\text{ML}}$ : indeed, we could take  $d = 1$ ,  $\tau = 2$ ,  $q = 1$  and  $p = 1/3$ , which yield  $a^{\text{SL}} \approx 1.75$  while  $a^{\text{ML}} = 2$  under  $k$ -orthogonality.

Now we compare with some multi-level MC and QMC works in the literature. Sometimes “finite-dimensional noise” is assumed, a feature we can mimic by setting  $p = q = 0$  in our analysis, leading to  $a^{\text{ML}} = \max(1/(1-\delta), d/\tau)$ . In [3, 5, 35], multi-level MC FE methods for elliptic PDEs (1) were analyzed, however with the random coefficient (2) being lognormal, i.e., the exponential of a stationary, Gaussian process.

In [26] a class of abstract multi-level QMC algorithms for infinite-dimensional integration was introduced, with a general cost model for the evaluation of the integrand function. The multi-level structure in that paper is different from ours: the key difference being that our multi-level scheme must also incorporate the multi-level structure of the FE discretizations. Also new is the necessity of considering ‘mixed’ regularity (in weighted reproducing kernel Hilbert spaces with respect to the parameter sequence  $\mathbf{y}$  and in the smoothness scale  $Z'$  with respect to the spatial variable  $\mathbf{x}$ ).

In [2] a multi-level MC FE method with finite dimensional noise was analyzed. It was shown there that in domains  $D \subset \mathbb{R}^2$ , a FE approximation of the expectation of the random solution with the convergence rate  $\mathcal{O}(h_L)$  in the norm of  $V$  (rather than for linear functionals of the solution) can be computed in  $\mathcal{O}(M_{h_L}) = \mathcal{O}(h_L^{-2})$  work and memory, i.e., with the same cost as one multi-level solution of the deterministic problem.

## 4 Conclusion

This paper introduces a multi-level QMC FE method, applied to functionals of the solution of the same PDE with random coefficient problem as considered by [6]. The same problem was studied by the present authors in [23], where we developed a single level QMC analysis which yielded the same error bounds as in [6] within the range of convergence rates relevant to QMC. The aim of the present multi-level version of the QMC approach is to develop a method which significantly reduces the costs, while maintaining the fast convergence (compared to MC) associated with QMC. We emphasize that the multi-level version requires a new analysis, and in particular leads

to a new prescription for the POD weights (different from that in [23]) that determine the QMC rule. Another difference is that the regularity requirements on the functions  $\psi_j$  are also more stringent than in the single level case.

The principal results for dimension  $d = 2$  are as follows. In Scenario 1 where  $k$ -orthogonality (28) holds, if we can choose  $t = t' = 1$  so that  $\tau = 2$ , and can choose  $\lambda = 1/(2 - 2\delta)$  for some  $\delta \in (0, 1/2)$ , then the cost of the multi-level QMC FE algorithm for computing the expectation of  $G(u)$  is  $\mathcal{O}(2^{2L/(1-\delta)}) = \mathcal{O}(h_L^{2/(1-\delta)})$ , while the convergence rate is the (best possible) second order  $\mathcal{O}(2^{-2L}) = \mathcal{O}(h_L^2)$ . This corresponds to optimal accuracy versus work bounds for the computation of solution functionals in first order FE methods applied to deterministic,  $H^2$  regular, second order elliptic problems (see, e.g. [4]). In contrast, multi-level MC FE methods such as those analyzed in [3, 5] cannot achieve optimal complexity for output functionals for general, sufficiently regular covariances of the random field  $a(\mathbf{x}, \mathbf{y})$ , due to the maximal convergence rate  $1/2$  of standard MC methods.

As noted earlier, our cost model does not include the pre-computation cost for the CBC construction of lattice rules. This is justified because the same lattice rules can be used for the PDE problem with different forcing terms  $f$ . However, as we are tailoring the choice of weights to the problem, the cost of the CBC construction may be a significant issue.

The present analysis was performed under Lipschitz assumptions on  $\psi_j$  and  $\bar{a}$  in (A4) and (A7) which, together with (A6) and the assumption that  $G(\cdot) \in L^2(D)$ , ensure in (6) that  $Z = (H_0^1 \cap H^2)(D)$  and, in turn, implies  $\mathcal{O}(h^2)$  convergence in (16). The present convergence analysis extends directly to weaker assumptions: if in (A4) and (A7) we have only Hölder continuity  $C^{0,r}(\bar{D})$  for some  $0 < r < 1$  instead of  $W^{1,\infty}(D)$  regularity, or if  $D$  is not convex, then  $\bar{b}_j$  in (35), (60) and (62) will depend on  $\|\psi_j\|_{C^{0,r}(\bar{D})}$  rather than on  $\|\psi_j\|_{W^{1,\infty}(D)}$ .

In Theorems 7 and 8 we considered only the weighted Sobolev space norm involving mixed first derivatives with respect to  $\mathbf{y}$ , but Theorem 6 holds for higher order mixed derivatives. The results here can be extended by considering higher order QMC methods, see e.g. [10, Chapter 15].

Finally, in our multi-level scheme we assumed that *exact expectations*  $\mathbb{E}[\cdot]$  with respect to random shifts  $\mathbf{\Delta}_\ell \in [0, 1]^{s_\ell}$  are available. In practical realizations, these expectations must be approximated by MC estimates  $E_{m_\ell}[\cdot]$  based on a finite number  $m_\ell$  of i.i.d. realizations of the shift  $\mathbf{\Delta}_\ell$  at discretization level  $\ell = 0, 1, \dots, L$ . This leads to a further error  $(\mathbb{E} - E_{m_\ell})[\cdot]$  in term  $\ell$  of (23) of order  $\mathcal{O}(m_\ell^{-1})$ . We can maintain our error-versus cost estimates in §3.7, with the same choices of parameters  $s_\ell$  and  $N_\ell$ , by taking  $m_\ell = m^*$  independent of  $\ell$ , that is, a level-independent, fixed number of random shifts  $\mathbf{\Delta}_\ell$  for each level  $\ell$ .

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