Report

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Multi-level quasi-Monte Carlo Finite Element methods for a class of elliptic PDEs with random coefficients

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Abstract This paper is a sequel to our previous work (Kuo, Schwab, Sloan, SIAM J. Numer. Anal., 2013) where quasi-Monte Carlo (QMC) methods (specifically, randomly shifted lattice rules) are applied to Finite Element (FE) discretizations of elliptic partial differential equations (PDEs) with a random coefficient represented in a countably infinite number of terms. We estimate the expected value of some linear functional of the solution, as an infinite-dimensional integral in the parameter space. Here the (single level) error analysis of our previous work 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 (i.e., the root-mean-square error averaged over all shifts) is of order $O(h^2)$, where $h$ is the finest FE mesh width, or $O(N^{-1+\delta})$ 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 essentially of the order of one single PDE solve at the finest FE discretization level, for spatial dimension $d = 2$ 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 variables (the parameters corresponding to randomness). As in our previous work, 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.

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1 Introduction

This paper is a sequel to our work [24], 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 [24], we consider the model parametric elliptic Dirichlet problem

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

for \( D \subset \mathbb{R}^d \) a bounded domain with a Lipschitz boundary \( \partial D \), where \( d = 1, 2, \) or \( 3 \) is assumed given and fixed (we do not track the dependence of constants on \( d \) in this work). In (1), the gradients are understood to be with respect to the physical variable \( x \) which belongs to \( D \), and the parameter vector \( y = (y_j)_{j \geq 1} \) consists of a countable number of parameters \( y_j \) which we assume, as in [24], to be i.i.d. uniformly distributed. Hence, we assume

\[ y \in [-\frac{1}{2}, \frac{1}{2}]^N =: U. \]

The parameter \( y \) is thus distributed on \( U \) with the uniform probability measure \( \mu(dy) = \otimes_{j \geq 1} dy_j = dy \). This simple probability model readily lends itself to treatment by QMC integration.

The parametric diffusion coefficient \( a(x,y) \) in (1) is assumed to depend linearly on the parameters \( y_j \) as follows:

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

The \( \psi_j \) can arise from either the eigensystem of a covariance operator (see, e.g. [32]), or other suitable function systems in \( L^2(D) \). As in [24] 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 \( 0 < a_{\min} \leq a(x,y) \leq a_{\max} \) for all \( x \in D \) and \( y \in U \).

(A3) There exists \( p \in (0,1) \) such that \( \sum_{j \geq 1} \| \psi_j \|_{L^p(D)}^p < \infty \).

(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 \( \| \psi_1 \|_{L^\infty(D)} \geq \| \psi_2 \|_{L^\infty(D)} \geq \cdots \).

(A6) The domain \( D \) is a convex and bounded polyhedron.
In this paper we impose one additional assumption:

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

We now briefly comment on each assumption. Assumption (A1) ensures that the coefficient \( a(x, y) \) is well-defined for all parameters \( y \in U \). Assumption (A2) yields the strong ellipticity needed for the standard FE analysis. Assumption (A3) is stronger than the second part of Assumption (A1). This assumption implies decay of the fluctuation coefficients \( \psi_j \), with faster decay for smaller \( p \). The value of \( p \) determines the convergence rate in the previous paper [24]. Assumption (A4) guarantees that the solutions converge to the solution of (1). 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. Assumption (A6) only simplifies the FE analysis and can be substantially relaxed. Finally, Assumption (A7) is often stronger than Assumptions (A3) and (A4). The value of \( q \in [p, 1] \) as well as that of \( p \in (0, 1) \) will determine the QMC convergence rates to be shown in this paper.

Our aim in this paper is to extend the QMC FE algorithm of [24] 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 continuous linear functional is \( G : H^1_0(D) \rightarrow \mathbb{R} \) (later we may impose stronger regularity assumption on \( G \), e.g., \( G \in L^2(D) \)). We are interested in approximating the integral

\[
I(G(u)) := \int_D G(u(\cdot, y)) \, dy := \lim_{s \to \infty} I_s(G(u)),
\]

where

\[
I_s(G(u)) := \int_{[-\frac{1}{s}, \frac{1}{s}]^d} G(u(\cdot, (y_1, \ldots, y_s, 0, 0, \ldots))) \, dy_1 \cdots dy_s.
\]

The (single level) strategy in [24] 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

\[
Q_{s,N}(G(u_s)) := \frac{1}{N} \sum_{j=1}^N G(u_s^{(j)}(\cdot, y^{(j)})),
\]

where \( u_s^{(j)} \) denotes the FE solution of the truncated PDE problem, and \( y^{(1)}, \ldots, y^{(N)} \) are QMC sample points which are judiciously chosen from the \( s \)-dimensional unit cube \( [-\frac{1}{s}, \frac{1}{s}]^d \). More precisely, the QMC rules considered in [24] are randomly shifted lattice rules; more details will be given in the next section. It was established in [24] that the root-mean-square of the error \( I(G(u)) - Q_{s,N}(G(u_s)) \) 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 \( f, G \in L^2(D) \), it was shown that the three additive parts of the error are of orders \( O(s^{-1}) \), \( O(N^{-1+\delta}) \), \( O(1) \).
and $\mathcal{O}(h^2) = \mathcal{O}(M^{-2/d}_h)$, 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 $\mathcal{O}(s N M_h)$. 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. In effect, we assume that the entries of the FE stiffness matrix can be computed exactly. The assessment of the impact of quadrature errors in the FE method is a classical problem, which is well studied and covered in texts, such as the monograph of Ciarlet [4].

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 [24]. The multi-level algorithm takes the form

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

(4)

where $\{s_{\ell}\}_{\ell \geq 0}$ is a nondecreasing sequence of truncation dimensions, $u_{s_{\ell}}^{h_{\ell}}$ 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 $u_{s_{-1}}^{h_{-1}} \equiv 0$, and $Q_{s, N}$ denotes the (randomly shifted) QMC quadrature rule with $N$ points in $s$ 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 $I(G(u)) - Q^L_s \left( G(u) \right)$ 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 [20] and reinvented by Giles [15, 16]. 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 [17, 27]. 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, 31, 36]. The model considered here, as in [24], is infinite-dimensional. Previous treatments of infinite-dimensional quadrature include [17, 25, 27] with QMC methods, [21] with MC methods, and [30] with Smolyak (or sparse-grid) quadrature. Applications of QMC methods to the “lognormal case” are considered in [18, 19].

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 $u^h_\ell = u_h$. Furthermore, due to the special structure of the expansion of the coefficient $a(x,y)$, the overall cost is only $O(\sum_{\ell=0}^{L} N_{\ell} M_{h,\ell} \log(M_{h,\ell}))$ 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 $x$ and to the parametric variable $y$. Another key point is that we require decay of stronger norms of the fluctuation coefficients $\psi_j$, see Assumption (A7). For the multi-level QMC FE algorithm, the convergence rate will be determined by both the values of $q$ in (A7) and $p$ in (A3), rather than just the value of $p$ as for the single level algorithm in [24]. 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 [24] 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”:

$$\gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j,$$

where $|u|$ denotes the cardinality (or the “order”) of the set $u$. These weights are then determined by the two sequences: by $\Gamma_0 = 1$, $\Gamma_1, \Gamma_2, \Gamma_3, \ldots$ and by $\gamma_1, \gamma_2, \gamma_3, \ldots$. The error bound obtained in the present paper is more complicated than the result in [24] 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 [24]. In any case, fast CBC construction algorithms for randomly shifted lattice rules are available for POD weights, see [10] or [23] for recent surveys, as well as [33, 22, 9, 28, 29, 7, 12].

The outline of this paper is as follows. In §2 we introduce the function spaces used for the analysis and summarize those results from [24] 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 [24] which will be used in what follows. Our variational setting of (1) is based on the Sobolev space $V = H^1_0(D)$ 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 \( x \),

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

with the norm

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

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 \( \phi_\lambda \in V \) and the eigenvalues \( \lambda \) in the corresponding spectrum \( \Sigma \) of the Dirichlet Laplacian in \( D \) by

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

Here, and in the following, we denote by \((\cdot, \cdot)\) the bilinear form corresponding to the \( L^2(D) \) inner product, extended by continuity to the duality pairing \( H'(D) \times H^{-1}(D) \). Standard elliptic regularity theory (see, e.g. [14]) yields the inclusion \( Z^t \subset H^1_{\text{loc}}(D) \), and for convex domains \( D \) and for \( t = 1 \) we have \( Z^1 = H^2(D) \cap H^1_0(D) \). As already seen in §1, we will also make use of the norm

\[
\|v\|_{W^{1,r}(D)} := \max\{\|v\|_{L^r(D)}, \|\nabla v\|_{L^r(D)}\}.
\]

The integrand in (3) is \( G(u(\cdot, y)) \). To analyze QMC integration for such integrands, we shall need a function space defined with respect to \( y \). Since our multi-level QMC FE algorithm makes use of the FE solution \( u_0^s \) of the truncated PDE problem to \( s \) terms, we consider the weighted and unanchored Sobolev space \( W_{s,y} \), which is a Hilbert space containing functions defined over the \( s \)-dimensional unit cube \([-\frac{1}{2}, \frac{1}{2}]^s\), with square integrable mixed first derivatives. More precisely, the norm for \( F = G(u_0^s) \in W_{s,y} \) is given by

\[
\|F\|_{W_{s,y}} := \left( \sum_{u \in \{1 : s\}} \frac{1}{\gamma_u} \int_{[-\frac{1}{2}, \frac{1}{2}]^s} \left| \int_{[-\frac{1}{2}, \frac{1}{2}]^s} \frac{\partial |u|}{\partial y_u} (y_{u, 1} - u_{1, 1}) \ dy_u \right|^2 dy_u \right)^{1/2},
\]

where \( \{1 : s\} \) is a shorthand notation for the set \( \{1, \ldots, s\} \), \( \frac{\partial |u|}{\partial y_u} \) denotes the mixed first derivative with respect to the “active” variables \( y_u = (y_j)_{j \in u} \), and where \( y_{-u} = (y_j)_{j \in \{1 : s\} \setminus u} \) denotes the “inactive” variables. The “outer” integration in (8) is omitted when \( u = \emptyset \), while the “inner” integration is omitted when \( u = \{1 : s\} \).

Weighted spaces were first introduced by Sloan and Woźniakowski in [34], and by now there are many variants, see e.g. [13, 35]. As in [24], we have taken the cube to be centered at the origin (rather than the standard unit cube \([0,1]^s\)). Moreover, we have adopted “general weights”: there is a weight parameter \( \gamma_u \) associated with each group of variables \( y_u = (y_j)_{j \in u} \) with indices belonging to the set \( u \), with the convention that \( \gamma_\emptyset = 1 \). Later we will focus on “POD weights”, see (5). As in [24], these POD weights arise naturally from our analysis for the PDE application.
2.2 Parametric Weak Formulation

As in [24], we consider the following parameter-dependent weak formulation of the parametric deterministic problem (1): for \( f \in V^* \) and \( y \in U \), find
\[
\mathbf{u}(\cdot, y) \in V : \quad b(y; \mathbf{u}(\cdot, y), v) = (f, v) \quad \forall v \in V ,
\]
where the parametric bilinear form \( b(y; w, v) \) is given by
\[
b(y; w, v) := \int_D a(x, y) \nabla w(x) \cdot \nabla v(x) \, dx , \quad \forall w, v \in V .
\]

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 apriori estimate. Moreover, additional regularity of the solution with respect to \( x \) can be obtained under additional regularity assumptions on \( f \) and the coefficients \( a(\cdot, y) \).

Theorem 1 ([24, Theorems 3.1 and 4.1]) Under Assumptions (A1) and (A2), for every \( f \in V^* \) and every \( y \in U \), there exists a unique solution \( \mathbf{u}(\cdot, y) \in V \) of the parametric weak problem (9), which satisfies
\[
\| \mathbf{u}(\cdot, y) \|_V \leq \frac{\| f \|_{V^*}}{a_{\min}} . \tag{10}
\]

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 \( y \in U \),
\[
\| \mathbf{u}(\cdot, y) \|_{Z^t} \leq C \| f \|_{H^{-1+t}(D)} , \tag{11}
\]
with the norm in \( Z^t \) defined by (7).

2.3 Dimension Truncation

Next we summarize a result from [24] needed for estimating the dimension truncation error. Given \( s \in \mathbb{N} \) and \( y \in U \), we observe that truncating the sum in (2) at \( s \) terms is the same as anchoring or setting \( y_j = 0 \) for \( j > s \). We denote by \( \mathbf{u}^t(x, y) := u(x, (y_{[1:s]}; 0)) \) 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 [24], it will be convenient for the regularity analysis of (1) and for the QMC error analysis to introduce
\[
b_j := \frac{\| \psi_j \|_{L^\infty(D)}}{a_{\min}} , \quad j \geq 1 . \tag{12}
\]

Theorem 2 ([24, Theorem 5.1]) Under Assumptions (A1) and (A2), for every \( f \in V^* \), every \( G \in V^* \), every \( y \in U \) and every \( s \in \mathbb{N} \), the solution \( \mathbf{u}^t(\cdot, y) = u(\cdot, (y_{[1:s]}; 0)) \) of the truncated parametric weak problem (9) satisfies, with \( b_j \) as defined in (12),
\[
\| \mathbf{u}(\cdot, y) - \mathbf{u}^t(\cdot, y) \|_V \leq C \frac{\| f \|_{V^*}}{a_{\min}} \sum_{j \geq r+1} b_j .
\]
of the parametric deterministic problem: for some constants \( C, \tilde{C} > 0 \) independent of \( s, f \) and \( G \). In addition, if Assumptions \( (A3) \) and \( (A5) \) hold, then

\[
\sum_{j \geq x+1} b_j \leq \min \left( \frac{1}{1/p-1}, 1 \right) \left( \sum_{j \geq 1} b_j^p \right)^{1/p} s^{(r-1/p-1)}.
\]  

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 \( T_h \) in \( D \) obtained from an initial, regular triangulation \( T_0 \) 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 \( h \to 0 \), with the norm in \( Z_t \) defined by (7),

\[
\inf_{v_h \in V_h} \|v - v_h\|_V \leq C h^r \|v\|_{Z_t} \quad \text{for all } v \in Z_t, \quad 0 \leq t \leq 1.
\]

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

\[
u \in V_h : \quad b(y, u_h(\cdot, y), v_h) = (f, v_h) \quad \forall v_h \in V_h.
\]

Below we summarize the results from [24] regarding the FE error. We remark that, by considering the error in approximating a bounded linear functional, \( O(h^2) \) convergence for \( f, G \in L^2(D) \) follows from an Aubin-Nitsche duality argument.

**Theorem 3** ([24, Theorems 7.1 and 7.2]) Under Assumptions \( (A1), (A2), (A4), \) and \( (A6) \), for every \( f \in V^* \) and every \( y \in U \), the FE approximations \( u_h(\cdot, y) \) are stable in the sense that

\[
\|u_h(\cdot, y)\|_V \leq \frac{\|f\|_{V^*}}{d_{\min}}.
\]

Moreover, for every \( f \in H^{-1+r}(D) \) with \( 0 \leq r \leq 1 \), every \( G \in H^{-1+r'}(D) \) with \( 0 \leq r' \leq 1 \), and for every \( y \in U \), there hold the asymptotic convergence estimates as \( h \to 0 \)

\[
\|u(\cdot, y) - u_h(\cdot, y)\|_V \leq C h^r \|u(\cdot, y)\|_{Z_t} \leq C h^r \|f\|_{H^{-1+r}(D)}
\]

and

\[
|G(u(\cdot, y)) - G(u_h(\cdot, y))| \leq \tilde{C} h^{r'} \|G\|_{H^{-1+r'}(D)} \|f\|_{H^{-1+r}(D)},
\]

where \( 0 \leq \tau := r + r' \leq 2 \), and where \( C, \tilde{C} > 0 \) are independent of \( h \) and \( y \).
2.5 QMC Approximation

As in [24], 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 $[-\frac{1}{2}, \frac{1}{2}]^s$,

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

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

$$Q_{s,N}(\Delta; F) := \frac{1}{N} \sum_{i=1}^{N} F \left( \frac{iz}{N} + \Delta \right) - \left( \frac{1}{N}, \ldots, \frac{1}{N} \right),$$

where $z \in \mathbb{Z}^s$ is known as the generating vector, which is deterministic, while $\Delta$ is the random shift to be drawn from the uniform distribution on $[0, 1]^s$, and $\frac{\cdot}{N} \lfloor \cdot \rfloor$ means to take the fractional part of each component in the vector. The subtraction by the vector $(\frac{1}{N}, \ldots, \frac{1}{N})$ describes the translation from the usual unit cube $[0, 1]^s$ to $[-\frac{1}{2}, \frac{1}{2}]^s$. For the weighted Sobolev space $\mathcal{W}_{s,\gamma}$ with POD weights, good generating vectors $z$ can be constructed, using a component-by-component algorithm at the cost of $O(sN \log N + s^2N)$ operations, such that the “shift averaged” worst case error achieves a dimension-independent convergence rate close to $O(N^{-1})$. Moreover, the implied constant in the big-$O$ bound can be independent of $s$ under appropriate conditions on the weights $\gamma_i$. A short summary of these results, together with references, can be found in [24, Section 2]. More detailed surveys can be found in [10] or [23]. For the purpose of this paper, we only need the following bound on the root-mean-square error.

**Theorem 4 ([24, Theorem 2.1])** Let $s, N \in \mathbb{N}$ be given, and assume $F \in \mathcal{W}_{s,\gamma}$ for a particular choice of weights $\gamma = (\gamma_i)$. 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 $\lambda \in (1/2, 1]$,

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

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

$$\rho(\lambda) := \frac{2\zeta(2\lambda)}{(2\pi^2)^\lambda},$$

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

For example, when $N$ is prime, $\phi(N) = N - 1$ and a rate of convergence arbitrarily close to $O(N^{-1})$ comes from taking $\lambda$ in the theorem close to $1/2$. However, note that $\rho(\lambda) \to 0$ as $\lambda \to (1/2)+$, making the convergence of the sum over $u$ 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

\[ h_\ell = 2^{-\ell} h_0 \quad \text{for} \quad \ell = 0, 1, 2, \ldots. \]

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

\[ M_{h_0} < M_{h_1} < \cdots < M_{h_\ell} := \dim(V_{h_\ell}) \approx 2^{d\ell} \rightarrow \infty \quad \text{as} \quad \ell \rightarrow \infty, \]

where \( a_n \approx b_n \) 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 \( \ell = 0, \ldots, L \) of (uniform) mesh refinement \( \mathcal{S}_\ell \) 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 \( \{s_\ell\}_{\ell = 0}^{\ell = L} \) of active dimensions is nondecreasing, i.e.,

\[ s_0 \leq s_1 \leq \cdots \leq s_\ell \leq s_L, \quad (18) \]

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

\[ V_\ell \equiv V_{h_\ell}, \quad \mathcal{S}_\ell \equiv \mathcal{S}_{h_\ell}, \quad Q_\ell \equiv Q_{s_\ell, N_\ell}, \quad I_\ell \equiv I_{s_\ell}, \quad u_\ell \equiv u_{h_\ell}^{s_\ell}, \quad M_\ell \equiv M_{h_\ell}. \]

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 \( u_{h_0}(y_{[1, s_\ell]}; 0) \). For convenience we define \( u_{-1} \equiv 0 \). Each lattice rule \( Q_\ell \) depends on a deterministic generating vector \( z_\ell \in \mathbb{Z}^{s_\ell} \), but we shall suppress this dependence in our notation. A realization of the lattice rule \( Q_\ell \) for a draw of the shift \( \Delta_\ell \in [0, 1]^{s_\ell} \) applied to a function \( F \) will be denoted by \( Q_\ell(\Delta_\ell; F) \). The random shifts \( \Delta_0, \ldots, \Delta_L \) 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

\[ Q^L(\Delta; G(u)) := \sum_{\ell=0}^{L} Q_\ell(\Delta_\ell; G(u_\ell - u_{\ell-1})), \quad (19) \]

where \( \Delta := (\Delta_0, \ldots, \Delta_L) \) will be referred to as the “compound shift”: it comprises all \( s_\ell := \sum_{\ell=0}^{L} s_\ell \) components of the random shifts \( \Delta_\ell \). Equivalently, \( \Delta_\ell \) is drawn from the uniform distribution over \([0, 1]^{s_\ell}\).

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 \( \Delta_\ell \), thus takes the form

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

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 $I$, $I_\ell$, $Q_l$ and $G$, we can express the error as

$$I(G(u)) - Q^G_\ell(\Delta; G(u)) = I(G(u)) - \sum_{\ell=0}^L I_\ell(G(u_\ell - u_{\ell-1})) = T_1 + T_2(\Delta_\ell),$$

where

$$T_1 := I(G(u)) - \sum_{\ell=0}^L I_\ell(G(u_\ell - u_{\ell-1})), \quad (21)$$

$$T_2(\Delta_\ell) := \sum_{\ell=0}^L (I_\ell - Q_\ell(\Delta_\ell))(G(u_\ell - u_{\ell-1})), \quad (22)$$

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 $\Delta_\ell \in [0,1]^d$, simplifies to

$$\mathbb{E}[|I(G(u)) - Q^G_\ell(\cdot; G(u))|^2] = T_1^2 + \mathbb{E}[T_2^2],$$

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

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

where the expectation inside the sum over index $\ell$ is with respect to the random shift $\Delta_\ell \in [0,1]^d$.

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

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

Here $u_{h_L} - u_{h_L}^L$ is the error that we incur in the FE approximation by omitting in the coefficient expansion (2) all terms with indices $j > s_\ell$. 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 $\theta_L \in \{0,1\}$, with $\theta_L = 1$ in general and $\theta_L = 0$ indicating that there is no truncation error, and arrive at the estimate

$$|T_1| \leq \sup_{y \in U} |G(u(\cdot, y) - u_{h_L}(\cdot, y))| + \theta_L |I(G(u_{h_L} - u_{h_L}^L))|$$

$$\leq C h_L^\delta \|f\|_{H^{1+\delta}(D)} \|g\|_{H^{1+\delta'}(D)} + \theta_L C \frac{\|f\|_{V^*} \|g\|_{V^*}}{\min_j b_j} \left( \sum_{j \geq s_L + 1} b_j \right)^2, \quad (24)$$

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

$$
\mathbb{E}[T^2_2] \leq \sum_{\ell=0}^{L} \left( \sum_{\ell' \leq \ell} \frac{\gamma^{1/\lambda}_{\ell}}{[\theta(\ell)]^{1/\lambda}} \right) \frac{1}{[\theta(\ell)]^{1/\lambda}} \|G(u^{\ell}_{h_\ell} - u^{\ell}_{h_{\ell-1}})\|_{L^2}^2.
$$

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

$$
\|G(u^{\ell}_{h_\ell} - u^{\ell}_{h_{\ell-1}})\|_{L^2} \leq \|G(u^{\ell}_{h_\ell} - u^{\ell}_{h_{\ell-1}})\|_{W^{s,1}} + \|G(u^{\ell}_{h_\ell} - u^{\ell}_{h_{\ell-1}})\|_{W^{s,1}}.
$$

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 $u^{s_{\ell}-1}_{h_{\ell-1}} = u^{s_{\ell}}_{h_{\ell-1}} = u_{h_{\ell-1}}$. This can happen when there is a special orthogonality property between the functions $\psi_j$ in the representation (2) and the FE spaces $V_j$. 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

$$
\{ \psi_j : j \geq 1 \} = \{ \psi^n_m : n \geq 0, m \in J_n \},
$$

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 $\psi^n_m$ 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 $|J_n| \geq 2^{dn}$.

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

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

$$
S^1(D, \mathcal{T}) := \{ v \in H^1_0(D) : v|_K \in P^1(K) \text{ for all } K \in \mathcal{T} \},
$$

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 $\{ \psi^n_m \}_{n \geq 0, m \in J_n}$ 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

$$
\int_{D} \psi^n_m(x) z_\ell(x) \, dx = 0 \quad \text{for all } n \geq \ell + k, \ m \in J_n, \text{ and } z_\ell \in S^0(D, \mathcal{T}_\ell),
$$

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

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

$$
\int_{D} \psi^n_m(x) \, dx = 0 \quad \text{for all } n \geq k \text{ and all } m \in J_n.
$$
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 $m = 0, \ldots, a - 1$,

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

and for $n \geq 1$,

$$\psi^n_m(x) := d^n_m \psi(2^n x - 2m), \quad m = 0, \ldots, 2^{n-1}a - 1,$$

where $d^n_m$ 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 $\{\psi^n_m\}$ forms an orthogonal basis of $L^2([0, a])$ if $d^n_m > 0$. We remark that the choice $d^n_m = 2^{(n-1)/2}$ which is well-known to imply orthonormality of the $\psi^0_m$ 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, $\ldots$, $a - 1$. 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, $\mathcal{R}_\ell$ 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 $\mathcal{R}_\ell$, the multiresolution sequence $\{\psi^n_m\}$ has the $k$-orthogonality property with respect to $\mathcal{R}_\ell$ with $k = 1$, for all $\ell \geq 0$. For example, for $\ell = 0$ and $n = 1, m = 0$ we have, with $z_0 \in S^0([0, a], \mathcal{R}_0)$ and $c := z_0[0,1]$,

$$\int_0^a \psi^1_0(x)z_0(x)\, dx = c \int_0^1 \psi^1_0(x)\, dx = c d^1_0 \int_0^1 \psi(2x)\, dx = 0.$$  

Haar wavelets do not satisfy Assumption (A4), since for (A4) to hold the basis functions $\psi^n_m$ 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, 26]; 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 $s_j$ is chosen appropriately at each level. This result is intrinsically linked to the linear structure in (2). To achieve this, we employ a one-to-one mapping of the indices between the functions $\psi_j$ and $\psi^n_m$ in (27): instead of ordering the functions as in Assumption (A5), we index $j$ according to a level-wise grouping so that the functions $\{\psi^0_m\}_{m \in J_0}$ come before the functions $\{\psi^1_0\}_{m \in J_1}$, followed by the functions $\{\psi^2_0\}_{m \in J_2}$, and so on. Correspondingly, we employ the same index mapping between $y_j$ and $y^n_m$ for the components of $y$.

**Theorem 5** Let $\{\psi^n_m : n \geq 0, m \in J_n\}$ be a multiresolution basis set for the domain $D$, with $|J_n| \approx 2^{dn}$, which has the $k$-orthogonality property with $k \in \{1, 2\}$ with respect to
the triangulations \( \{ T_\ell : \ell \geq 0 \} \). Let \( \{ y_j : j \geq 1 \} = \{ y_m^n : n \geq 0, m \in J_n \} \) denote the corresponding parameters under the level-wise relabelling (27) so that the parametric coefficient in (2) can be represented in the form

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

Let

\[
s_\ell := \sum_{n=0}^{\ell+k-1} |J_n|.
\]

Then \( s_\ell \geq 2^{d\ell} \geq M_{hi} \), and for all \( \ell \geq 0 \) we have

\[
u_{hi} = u_{hi}^{s_\ell}.
\]

As \( \ell \to \infty \), the number of nonzero entries in the Finite Element stiffness matrix for the parametric coefficient \( a(x, y) \) at meshlevel \( \ell \geq 0 \) for any given \( y \in U \) is \( \mathcal{O}(M_{hi}) \). We assume that each of the nonzero entries can be computed in \( \mathcal{O}(\log(M_{hi})) \) operations, leading to a total cost of \( \mathcal{O}(M_{hi} \log(M_{hi})) \) operations.

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

\[
b(y; w_\ell, v_\ell) = \int_D \left( \bar{a}(x) + \sum_{n=0}^\infty \sum_{m \in J_n} y_m^n \psi_m^n(x) \right) \nabla w_\ell \cdot \nabla v_\ell \, dx
\]

\[
= \int_D \left( \bar{a}(x) + \sum_{n=0}^{\ell+k-1} \sum_{m \in J_n} y_m^n \psi_m^n(x) \right) \nabla w_\ell \cdot \nabla v_\ell \, dx
\]

\[
= b(y_{\{1,\ldots,\ell\}}; w_\ell, v_\ell).
\]

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

To show the assertion on the cost, for given \( y \) we denote by \( B^i(y) \) the \( M_i \times M_i \) stiffness matrix of the parametric bilinear form \( b(y; \cdot, \cdot) \), restricted to \( V_i \times V_i \), where \( V_i = \text{span}\{ \Phi_i^\ell : 1 \leq \ell \leq M_i \} \), 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 \( 1 \leq i, i' \leq M_i = \dim(V_i) = \mathcal{O}(2^{d\ell}) \) there holds

\[
B^i_i(y) = b(y_{\{1,\ldots,\ell\}}; \Phi_i^\ell, \Phi_i^\ell) = \int_D (P_{i+k-1} \bar{a}(x,y)) \nabla \Phi_i^\ell \cdot \nabla \Phi_i^\ell \, dx,
\]

where \( P_{i+k-1} \bar{a}(x,y) \) denotes the truncated expression for \( \bar{a}(x,y) \) appearing in (31). The matrix \( B^i(y) \) 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 \( \mathcal{O}(M_i) \) nonvanishing entries (32).

Now consider the cost for the exact evaluation of any matrix entry \( (B^i(y))_{i'i'} \neq 0 \). 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 \( \int_D \psi_m^n(x) \nabla \Phi_i^\ell \cdot \nabla \Phi_i^\ell \, dx \neq 0 \). Thus the cost for evaluating \( (B^i(y))_{i'i'} \neq 0 \) is \( \mathcal{O}(\ell + k - 1) \), which yields that the total cost for evaluating the sparse matrix is \( \mathcal{O}(M_i \ell) = \mathcal{O}(M_i \log(M_i)) \) operations.
3.4 Key Results

In the error analysis of the (single level) QMC FE method, we established in [24] 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 $x$ and $y$. 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 $\mathbf{v} = (v_j)_{j \geq 1} \in \mathbb{N}_0^j$, where $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$, we define $|\mathbf{v}| := v_1 + v_2 + \cdots$, and we refer to $\mathbf{v}$ as a “multi-index” and $|\mathbf{v}|$ as the “length” of $\mathbf{v}$. By

$$\tilde{\mathcal{S}} := \{ \mathbf{v} \in \mathbb{N}_0^j : |\mathbf{v}| < \infty \}$$

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 $\mathbf{v} \in \tilde{\mathcal{S}}$ we denote the partial derivative of order $\mathbf{v} \in \tilde{\mathcal{S}}$ of $u$ with respect to $y$ by

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

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

$$\|\partial_\mathbf{v}^y u(\cdot, y)\|_V \leq |\mathbf{v}|! \left( \prod_{j=1}^{34} b_j^{v_j} \right) \|f\|_{V^*} \frac{\alpha_{\min}}{\alpha_{\min}},$$  

(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

$$\|\partial_\mathbf{v}^y u(\cdot, y)\|_{V^*} \leq C|\mathbf{v}|! \left( \prod_{j=1}^{35} \tilde{b}_j^{v_j} \right) \|f\|_{H^{-1+t}(D)},$$  

(34)

where

$$\tilde{b}_j := b_j + \kappa \gamma \left( \|\nabla \psi_j\|_{L^\infty(D)} + B \|\psi_j\|_{L^\infty(D)} \right), \quad j \geq 1,$$

(35)

and the constants $B$ and $C_1$ are, for $0 \leq t \leq 1$, defined by

$$B := \frac{1}{\alpha_{\min}} \sup_{z \in U} \|\nabla u(\cdot, z)\|_{L^\infty(D)} < \infty, \quad C_1 := \sup_{w \in L^2(D)} \|w\|_{H^{-1+t}(D)} < \infty.$$  

(36)

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

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

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

(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 $v(x) = \partial_y^\nu u(x, y) \in V$ in (37) leads to

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

(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 [24, Theorem 4.1]. To obtain the bounds for $|\mathbf{v}| \neq 0$, we observe that, trivially, for every $\mathbf{v} \in \mathfrak{F}$ and every $y \in U$, the function $\partial_y^\nu u(\cdot, y)$ is the solution of the Dirichlet problem

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

(39)

with

$$g_\nu(\cdot, y) := -\nabla \cdot (a(\cdot, y) \nabla (\partial_y^\nu u(\cdot, y))) = \nabla a(\cdot, y) \cdot \nabla (\partial_y^\nu u(\cdot, y)) + a(\cdot, y) \Delta (\partial_y^\nu u(\cdot, y)).$$

Here, we used the identity

$$\nabla \cdot (\alpha(x) \nabla w(x)) = \alpha(x) \Delta w(x) + \nabla \alpha(x) \cdot \nabla w(x),$$  

(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

$$\|\partial_y^\nu u(\cdot, y)\|_V \leq C \|g_\nu(\cdot, y)\|_{H^{-1+\epsilon}(D)}.$$  

(41)

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

$$|\langle g_\nu(\cdot, y), v \rangle| = |\langle \nabla \cdot (a(\cdot, y) \nabla (\partial_y^\nu u(\cdot, y))), v \rangle|$$

$$= \left| \sum_{j \in \text{supp}(\mathbf{v})} v_j \left( \nabla \psi_j \cdot \nabla (\partial_y^{\nu - \mathbf{e}_j} u(\cdot, y)) + \psi_j \Delta (\partial_y^{\nu - \mathbf{e}_j} u(\cdot, y)), v \right) \right|$$

$$\leq \sum_{j \in \text{supp}(\mathbf{v})} v_j \left\| \nabla \psi_j \cdot \nabla (\partial_y^{\nu - \mathbf{e}_j} u(\cdot, y)) + \psi_j \Delta (\partial_y^{\nu - \mathbf{e}_j} u(\cdot, y)) \right\|_{H^{-1+\epsilon}(D)} \|v\|_{H^{1-\epsilon}(D)}.$$

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

$$\|g_\nu(\cdot, y)\|_{H^{-1+\epsilon}(D)} \leq \sum_{j \in \text{supp}(\mathbf{v})} v_j \left( \|\nabla \psi_j\|_{L^\infty(D)} \left\| \nabla (\partial_y^{\nu - \mathbf{e}_j} u(\cdot, y)) \right\|_{H^{-1+\epsilon}(D)} + \|\psi_j\|_{L^\infty(D)} \|\Delta (\partial_y^{\nu - \mathbf{e}_j} u(\cdot, y))\|_{H^{-1+\epsilon}(D)} \right).$$  

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

$$-a(\cdot,y)\Delta(\partial_y^V e_j u(\cdot,y)) = \nabla a(\cdot,y) \cdot \nabla (\partial_y^V e_j u(\cdot,y)) - g_{\mathbf{v} - e_j}(\cdot,y), \tag{43}$$

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

$$||\Delta(\partial_y^V e_j u(\cdot,y))||_{H^{-1+1}(D)} \leq \frac{1}{a_{\min}}||\text{RHS of (43)}||_{H^{-1+1}(D)}\leq \frac{1}{a_{\min}} \left[\left(\sup_{z \in U} ||\nabla a(\cdot,z)||_{L^2(D)}\right) ||\nabla(\partial_y^V e_j u(\cdot,y))||_{H^{-1+1}(D)} + ||g_{\mathbf{v} - e_j}(\cdot,y)||_{H^{-1+1}(D)}\right] \leq B C \|\partial_y^V e_j u(\cdot,y)\|_V + \frac{1}{a_{\min}} \|g_{\mathbf{v} - e_j}(\cdot,y)\|_{H^{-1+1}(D)},$$

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

$$||g_{\mathbf{v}}(\cdot,y)||_{H^{-1+1}(D)} \leq \sum_{j \in \text{supp}(\mathbf{v})} v_j \left[C \left(||\nabla \psi_j||_{L^2(D)} + B \|\psi_j\|_{L^2(D)} \right) ||\partial_y^V e_j u(\cdot,y)\|_V + b_j \|g_{\mathbf{v} - e_j}(\cdot,y)\|_{H^{-1+1}(D)}\right] \tag{44}.$$ 

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

$$||\partial_y^V u(\cdot,y)||_V + \kappa ||g_{\mathbf{v}}(\cdot,y)||_{H^{-1+1}(D)} \leq \sum_{j \in \text{supp}(\mathbf{v})} v_j b_j \left[||\partial_y^V e_j u(\cdot,y)\|_V + \kappa \|g_{\mathbf{v} - e_j}(\cdot,y)\|_{H^{-1+1}(D)}\right] + \sum_{j \in \text{supp}(\mathbf{v})} v_j \kappa C \left(||\nabla \psi_j||_{L^2(D)} + B \|\psi_j\|_{L^2(D)} \right) ||\partial_y^V e_j u(\cdot,y)\|_V \leq \sum_{j \in \text{supp}(\mathbf{v})} v_j \tilde{b}_j \left[||\partial_y^V e_j u(\cdot,y)\|_V + \kappa \|g_{\mathbf{v} - e_j}(\cdot,y)\|_{H^{-1+1}(D)}\right], \tag{45}$$

where $\tilde{b}_j$ is as in (35). By Assumption (A4), we have $\sum_{j \geq 1} \tilde{b}_j < \infty$ 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 $\{\tilde{b}_j\}$ in place of $\{b_j\}$. For $|\mathbf{v}| = 0$, we find using (10) of Theorem 1 and $g_0 = -f$ that

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

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

$$\kappa ||g_{\mathbf{v}}(\cdot,y)||_{H^{-1+1}(D)} \leq ||\partial_y^V u(\cdot,y)||_V + \kappa ||g_{\mathbf{v}}(\cdot,y)||_{H^{-1+1}(D)} \leq |\mathbf{v}|! \left(\prod_{j \geq 1} \tilde{b}_j^V \right) \left(\frac{\tilde{C}}{a_{\min}} + \kappa \right) ||f||_{H^{-1+1}(D)}.$$
where \( \mathcal{C}_t := \sup_{w \in H^{-1+t}(D)} (\|w\|_{H^{-1}(D)}/\|w\|_{H^{-1+t}(D)}) < \infty \). Now (34) follows from (41).

To bound the first term in (26) we need Theorem 7 below. We shall make use of the following lemma which can be proved by induction. We use the convention that an empty product is 1.

**Lemma 1** Given non-negative numbers \((\beta_j)_{j \in \mathbb{N}}\), let \((A_\nu)_{\nu \subset \mathbb{N}}\) and \((B_\nu)_{\nu \subset \mathbb{N}}\) be non-negative real numbers satisfying the inequality

\[
A_\nu \leq \sum_{k \in \nu} \beta_k A_{\nu \setminus \{k\}} + B_\nu \quad \text{for any } \nu \subset \mathbb{N} \text{ (including } \nu = \emptyset) .
\]

Then we have

\[
A_\nu \leq \sum_{m \leq \nu} |m|! \left( \prod_{j \in \mathbb{N}} \beta_j \right) B_{\nu \setminus m} .
\]

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

\[
\|G(u^k - u^k_h)\|_{W^{s,T}} \leq C h^\kappa \alpha_{\max} \|f\|_{H^{-1+t}(D)} \|G\|_{H^{-1+t'}(D)} \left( \sum_{u \in \mathbb{N} \setminus \{1\}} \frac{[(u + 3)!]^2 \prod_{j \in \mathbb{N}} \tilde{b}_j^2}{\gamma_u} \right)^{1/2},
\]

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

**Proof** Let \( g \in H^{-1+t'}(D) \) denote the representor of \( G \in H^{-1+t'}(D) \). Here, for \( 0 < t' < 1 \), we have \( H^{-1+t'}(D) = (H^{-1+t'}_0(D))^* \) with duality taken with respect to the “pivot” space \( L^2(D) \simeq (L^2(D))^* \), and with \( H^{1-t'}_0(D) := (H^1_0(D), L^2(D))_{1-t'} \) defined by interpolation. Then, with \((\cdot, \cdot)\) denoting the \( H^{-1+t'}(D) \times H^{1-t'}_0(D) \) duality pairing, we have that \( G(w) = (g, w) \) for \( w \in H^{1-t'}_0(D) \).

For all \( y \in U \), we then define \( v^g(\cdot, y) \in V \) and \( v^h(\cdot, y) \in V_h \) by

\[
b(y, w, v^g(\cdot, y)) = (g, w) \quad \forall w \in V ,
\]

\[
b(y, w_h, v^h(\cdot, y)) = (g, w_h) \quad \forall w_h \in V_h ,
\]

so that \( v^g \) and \( v^h \) are the exact and FE solutions if \( f \) is replaced by \( g \). Taking \( w = u(\cdot, y) - u_h(\cdot, y) \), we have

\[
G(u(\cdot, y) - u_h(\cdot, y)) = (g, u(\cdot, y) - u_h(\cdot, y)) = b(y, u(\cdot, y) - u_h(\cdot, y), v^g(\cdot, y)) = b(y, u(\cdot, y) - u_h(\cdot, y), v^h(\cdot, y) - v^g(\cdot, y)) ,
\]

where we used Galerkin orthogonality \( b(y, u(\cdot, y) - u_h(\cdot, y), v^h(\cdot, y)) = 0 \).
Using the definitions of the bilinear form $b(y, \cdot, \cdot)$ and the norm $\|\cdot\|_{y,b}$, we obtain

$$
\|G(u' - u'_h)\|_{y,b} = \left( \sum_{u \in \{(1,\ldots,1)\}} \frac{1}{2^n} \int_{[-\frac{1}{2},\frac{1}{2}]^n} \left| \int_{[-\frac{1}{2},\frac{1}{2}]^n} r_u(y_u; y_u - u'_h) \, dy_u \right|^2 \, dy_u \right)^{1/2},
$$

where we define for all $y \in U$

$$
r_u(y) := \int_D \frac{\partial u|_{y_u}}{\partial y_u} \left( a(x,y) \nabla (u - u_h)(x,y) \cdot \nabla (v^\delta - v_h^\delta)(x,y) \right) \, dx.
$$

For the remainder of this proof, we will use the short-hand notation $\partial_u$ for the mixed first partial derivatives with respect to the variables $y_j$ for $j \in u$. From the definition of $a(x,y)$ we see that

$$
r_u(y) = \int_D a(x,y) \, \partial_u \left( \nabla (u - u_h)(x,y) \cdot \nabla (v^\delta - v_h^\delta)(x,y) \right) \, dx
$$

$$
+ \sum_{k \in u} \int_D \psi_k(x) \, \partial_u \left( \nabla (u - u_h)(x,y) \cdot \nabla (v^\delta - v_h^\delta)(x,y) \right) \, dx
$$

$$
+ \sum_{k \in u} \int_D \psi_k(x) \, \sum_{v \subseteq u \setminus \{k\}} \nabla \partial_u (u - u_h)(x,y) \cdot \nabla \partial_u (v^\delta - v_h^\delta)(x,y) \, dx,
$$

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

$$
|r_u(y)| \leq a_{\text{max}} \sum_{v \subseteq u} \|\partial_u (u - u_h)(\cdot,y)\|_V \|\partial_{u \setminus v} (v^\delta - v_h^\delta)(\cdot,y)\|_V
$$

$$
+ \sum_{k \in u} \|\psi_k\|_{L^\infty(D)} \sum_{v \subseteq u \setminus \{k\}} \|\partial_u (u - u_h)(\cdot,y)\|_V \|\partial_{u \setminus v} (v^\delta - v_h^\delta)(\cdot,y)\|_V.
$$

To continue, we need to obtain an estimate for $\|\partial_u (u - u_h)(\cdot,y)\|_V$. Let $I : V \to V$ denote the identity operator, and for $y \in U$ let $P_h = P_h(y) : V \to V_h$ denote the parametric FE projection defined by

$$
b(y; P_h w, z_h) = b(y; w, z_h) \quad \forall w \in V, \quad z_h \in V_h.
$$

Then we have $u_h = P_h u \in V_h$ and $\partial_u u_h \in V_h$, and hence $(I - P_h)\partial_u u_h = 0$. Thus

$$
\|\partial_u (u - u_h)(\cdot,y)\|_V = \|P_h \partial_u (u - u_h)(\cdot,y) + (I - P_h) \partial_u u(\cdot,y)\|_V
$$

$$
\leq \|P_h \partial_u (u - u_h)(\cdot,y)\|_V + \|(I - P_h) \partial_u u(\cdot,y)\|_V.
$$

Recall that Galerkin orthogonality gives $b(y; u(\cdot,y) - u_h(\cdot,y), z_h) = 0$ for all $z_h \in V_h$. Upon differentiating with respect to $y$ and $\partial_u$, we obtain for all $z_h \in V_h$

$$
\int_D a(x,y) \, \nabla \partial_u (u - u_h)(x,y) \cdot \nabla z_h(x) \, dx
$$

$$
= - \sum_{k \in u} \int_D \psi_k(x) \, \nabla \partial_{u \setminus \{k\}} (u - u_h)(x,y) \cdot \nabla z_h(x) \, dx.
$$
Using again the definition (48) of $\mathcal{P}_h$, we may replace $\partial_y(u-u_h)$ on the left-hand side of (50) by $\partial_y\mathcal{P}_h(u-u_h)$, we then obtain
\[
a_{\min} \|\mathcal{P}_h \partial_y (u-u_h) (\cdot, y)\|_V^2 \\
\leq \sum_{k \in \mathcal{D}} \| \psi_k \|_{L^\infty (D)} \| \partial_{\mathcal{P}_h \setminus \{ k \}} (u-u_h) (\cdot, y) \|_V \| \mathcal{P}_h \partial_y (u-u_h) (\cdot, y) \|_V,
\]
which in turn yields
\[
\| \mathcal{P}_h \partial_y (u-u_h) (\cdot, y) \|_V \leq \sum_{k \in \mathcal{D}} b_k \| \partial_{\mathcal{P}_h \setminus \{ k \}} (u-u_h) (\cdot, y) \|_V.
\]
(51)

Substituting (51) into (49) gives
\[
\| \partial_y (u-u_h) (\cdot, y) \|_V \leq \sum_{m \subseteq \mathcal{D}} \| m \| \left( \prod_{k \in \mathcal{D}} b_k \right) \| (\mathcal{I} - \mathcal{P}_h) \partial_{\mathcal{P}_h \setminus m} u (\cdot, y) \|_V,
\]
from which we conclude using Lemma 1 that
\[
\| \partial_y (u-u_h) (\cdot, y) \|_V \leq \sum_{m \subseteq \mathcal{D}} \| m \| \left( \prod_{k \in \mathcal{D}} b_k \right) \| (\mathcal{I} - \mathcal{P}_h) \partial_{\mathcal{P}_h \setminus m} u (\cdot, y) \|_V.
\]
Next we use the FE estimate that for all $y \in U$ and $w \in V$ we have $\| (\mathcal{I} - \mathcal{P}_h (y)) w \|_V \leq C h^T \| w \|_Z$ (in particular, this implies (15) in Theorem 3). This yields
\[
\| \partial_y (u-u_h) (\cdot, y) \|_V \leq C h^T \sum_{m \subseteq \mathcal{D}} \| m \| \left( \prod_{k \in \mathcal{D}} b_k \right) \| \partial_{\mathcal{P}_h \setminus m} u (\cdot, y) \|_Z
\]
\[
\leq C h^T \| f \|_{H^ {-1+\ell} (D)} \sum_{m \subseteq \mathcal{D}} \| m \| \left( \prod_{k \in \mathcal{D}} b_k \right) \| v \|_Z \left( \prod_{j \in \mathcal{D} \setminus m} b_j \right)
\]
\[
\leq C h^T \| f \|_{H^ {-1+\ell} (D)} (|v| + 1)! \prod_{j \in \mathcal{D}} b_j,
\]
(52)

where the second inequality follows from (34) in Theorem 6, and the final step follows from $b_k \leq \bar{b}_k$ and the identity $\sum_{m \subseteq \mathcal{D}} \| m \| \| v \setminus m \| = (|v| + 1)$. Throughout, $C > 0$ denotes a generic constant.

Similarly, with $f$ replaced by $g$, $u$ replaced by $v^g$, $u_h$ replaced by $v^g_h$, $t$ replaced by $t'$, and $v$ replaced by $u \setminus v$, we obtain
\[
\| \partial_{u \setminus v} (v^g - v^g_h) (\cdot, y) \|_V \leq C h^T \| g \|_{H^ {-1+\ell'} (D)} (|u \setminus v| + 1)! \prod_{j \in u \setminus v} b_j.
\]
(53)

Using (52) and (53) and the identity $\sum_{v \subseteq u} (|v| + 1)! (|u \setminus v| + 1)! = (|u| + 3)!/6$, we obtain from (47)
\[
|r_u (y)| \leq C h^T \| f \|_{H^ {-1+\ell} (D)} \| g \|_{H^ {-1+\ell'} (D)} \frac{1}{3} (|u| + 3)! \prod_{j \in u} b_j
\]
\[
+ C h^T \| f \|_{H^ {-1+\ell} (D)} \| g \|_{H^ {-1+\ell'} (D)} \sum_{k \in \mathcal{D}} \| \psi_k \|_{L^\infty (D)} \frac{1}{3} (|u| + 3)! \prod_{j \in u \setminus \{ k \}} b_j
\]
\[
\leq C h^T \| f \|_{H^ {-1+\ell} (D)} \| G \|_{H^ {-1+\ell'} (D)} (|u| + 3)! \prod_{j \in u} b_j,
\]
where we used the estimate $\| \psi_k \|_{L^\infty (D)} = a_{\min} b_k \leq a_{\max} \bar{b}_k$. Substituting this estimate into (46) completes the proof. \qed
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 \( G \in V^* \), every \( h > 0 \), and every \( \ell \geq 1 \),

\[
\|G(u_h^\ell - u_h^{\ell-1})\|_{W_{\ell, Y}} 
\leq \frac{\|f\|_{V^*} \|G\|_{V^*}}{\alpha_{\text{min}}} \left[ \left( \frac{1}{2} \sum_{j=s_{\ell-1}+1}^{s_\ell} b_j \right)^2 \sum_{u \subseteq \{1:s_{\ell-1}\}} \frac{[(|u| + 1)!]^2 \prod_{j \in u} b_j^2}{\gamma_u} \right]^{1/2} 
+ \frac{\sum_{u \subseteq \{1:s_{\ell-1}\}} \frac{[(|u| + n)!]^2 \prod_{j \in u} b_j^2}{\gamma_u}}{w^{s_{\ell-1}} \cap \{ \gamma_u \neq 0 \}} \right)^{1/2},
\]

(54)

where \( b_j \) is defined in (12). In addition, if \( s_{\ell-1} \neq s_\ell \), and Assumptions (A3) and (A5) hold, and the weights \( \gamma_u \) are such that

\[
\sum_{u \subseteq \{1:s_{\ell-1}\}} \frac{[(|u|)!]^2 \prod_{j \in u} b_j^2}{\gamma_u} \leq C s_{\ell-1}^{2\alpha} \sum_{u \subseteq \{1:s_{\ell-1}\}} \frac{[(|u| + n)!]^2 \prod_{j \in u} b_j^2}{\gamma_u}
\]

(55)

for some \( \alpha > 0 \) and integer \( n \geq 1 \), then

\[
\|G(u_h^\ell - u_h^{\ell-1})\|_{W_{\ell, Y}} 
\leq \tilde{C} \|f\|_{V^*} \|G\|_{V^*} s_{\ell-1}^{\min(1/p-1, \alpha)} \left( \sum_{u \subseteq \{1:s_{\ell-1}\}} \frac{[(|u| + n)!]^2 \prod_{j \in u} b_j^2}{\gamma_u} \right)^{1/2}.
\]

(56)

Both \( C, \tilde{C} > 0 \) are generic constants which are independent of \( s_\ell \) and \( s_{\ell-1} \).

**Proof** As in the proof of Theorem 7, we will use the short-hand notation \( \partial_u \) for the mixed first partial derivatives with respect to the variables \( y_j \) for \( j \in u \). For any \( y \in U \), \( u_h^{\ell}(\cdot, y) \) and \( u_h^{\ell-1}(\cdot, y) \) are the solutions of the variational problems:

\[
(a^{\ell}(\cdot, y) \nabla u_h^{\ell}(\cdot, y), \nabla z_h) = (f, z_h) \quad \forall z_h \in V_h, 
\]

(57)

\[
(a^{\ell-1}(\cdot, y) \nabla u_h^{\ell-1}(\cdot, y), \nabla z_h) = (f, z_h) \quad \forall z_h \in V_h.
\]

(58)

To estimate \( \|G(u_h^\ell - u_h^{\ell-1})\|_{W_{\ell, Y}} \), we make use of the inequality

\[
|\partial_u(G(u_h^\ell - u_h^{\ell-1})(y))| \leq \|G\|_{V^*} \|\partial_u(u_h^\ell - u_h^{\ell-1})(\cdot, y)\|_{V^*}.
\]

If \( u \cap \{s_{\ell-1}+1 : s_\ell\} \neq \emptyset \), then it follows from (33) of Theorem 6 that

\[
\|\partial_u(u_h^\ell - u_h^{\ell-1})(\cdot, y)\|_{V^*} = \|\partial_u u_h^\ell(\cdot, y)\|_{V^*} \leq |u|! \left( \prod_{j \in u} b_j \right) \frac{\|f\|_{V^*}}{\alpha_{\text{min}}}.
\]

(59)
On the other hand, if \( u \subseteq \{ 1 : s_{k-1} \} \) then we subtract (58) from (57) to obtain the equation \((a'^{\tau}(\cdot, y) \nabla u_{h}^{\tau}(\cdot, y) - a'^{\tau-1}(\cdot, y) \nabla u_{h}^{\tau-1}(\cdot, y), \nabla z_{h}) = 0\) for all \( z_{h} \in V_{h} \), or equivalently,
\[
(a'^{\tau}(\cdot, y) \nabla (u_{h}^{\tau}(\cdot, y) - u_{h}^{\tau-1}(\cdot, y)), \nabla z_{h}) = -((a'^{\tau}(\cdot, y) - a'^{\tau-1}(\cdot, y) \nabla u^{\tau-1}_{h}(\cdot, y), \nabla z_{h}) \quad \forall z_{h} \in V_{h}.
\]

Upon differentiating with respect to \( y_{u} \) for \( u \subseteq \{ 1 : s_{k-1} \} \), we obtain
\[
\int_{D} a'^{\tau}(x, y) \nabla \partial_{u}(u_{h}^{\tau} - u_{h}^{\tau-1})(x, y) \cdot \nabla z_{h}(x) \, dx
= -\sum_{k \subseteq u} \int_{D} \psi_{k}(x) \nabla \partial_{u \setminus \{ k \}}(u_{h}^{\tau} - u_{h}^{\tau-1})(x, y) \cdot \nabla z_{h}(x) \, dx
- \int_{D} \sum_{j = s_{k-1} + 1}^{s_{k}} \psi_{j}(x, y)_{j} \nabla \partial_{u} u^{\tau-1}_{h}(x, y) \cdot \nabla z_{h}(x) \, dx.
\]

Taking \( z_{h} = \partial_{u}(u_{h}^{\tau} - u_{h}^{\tau-1})(\cdot, y) \), we get using similar steps to those for obtaining (51),
\[
\| \partial_{u}(u_{h}^{\tau} - u_{h}^{\tau-1})(\cdot, y) \|_{V}
\leq \sum_{k \subseteq u} b_{k} \| \partial_{u \setminus \{ k \}}(u_{h}^{\tau} - u_{h}^{\tau-1})(\cdot, y) \|_{V} + \left( \frac{1}{2} \sum_{j = s_{k-1} + 1}^{s_{k}} b_{j} \right) \| \partial_{u} u^{\tau-1}_{h}(\cdot, y) \|_{V}.
\]

It then follows from Lemma 1 that
\[
\| \partial_{u}(u_{h}^{\tau} - u_{h}^{\tau-1})(\cdot, y) \|_{V}
\leq \left( \frac{1}{2} \sum_{j = s_{k-1} + 1}^{s_{k}} b_{j} \right) \| \partial_{u \setminus \{ k \}}(u_{h}^{\tau} - u_{h}^{\tau-1})(\cdot, y) \|_{V}
\leq \left( \frac{1}{2} \sum_{j = s_{k-1} + 1}^{s_{k}} b_{j} \right) \left( |u| ! \left( \prod_{j \in \emptyset} b_{j} \right) \sum_{v \subseteq u \setminus \emptyset} |v| ! |u \setminus v| ! \left( \prod_{j \in v} b_{j} \right) \frac{\| f \|_{v}}{a_{\min}} \right)^{2},
\]
where we used again (33) of Theorem 6 and the identity \( \sum_{v \subseteq u} |v| ! |u \setminus v| ! = (|u| + 1)! \).

Combining (59) and (60), we conclude that
\[
\| G(u_{h}^{\tau} - u_{h}^{\tau-1}) \|^{2}_{V_{\text{loc}}}
\leq \sum_{u \subseteq \{ 1 : s_{k-1} \}} \frac{1}{L_{u}} \left[ \| G \|_{V^{+}} \left( \frac{1}{2} \sum_{j = s_{k-1} + 1}^{s_{k}} b_{j} \right) (|u| + 1)! \left( \prod_{j \in u} b_{j} \right) \frac{\| f \|_{V^{+}}}{a_{\min}} \right]^{2}
+ \sum_{u \subseteq \{ 1 : s_{k-1} \}} \frac{1}{L_{u}} \left[ \| G \|_{V^{+}} |u| ! \left( \prod_{j \in u} b_{j} \right) \frac{\| f \|_{V^{+}}}{a_{\min}} \right]^{2},
\]
which yields the estimate (54). The estimate (56) then follows directly from (14) and the condition (55).
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

\[
\|G(u_{h_{\ell}}^{\ell} - u_{h_{\ell-1}}^{\ell})\|_{\mathcal{W}_{\gamma} \mathcal{T}} \leq \|G(u_{h_{\ell}}^{\ell} - u_{h_{\ell-1}}^{\ell})\|_{\mathcal{W}_{\gamma} \mathcal{T}} + \|G(u_{h_{\ell}}^{\ell} - u_{h_{\ell-1}}^{\ell})\|_{\mathcal{W}_{\gamma} \mathcal{T}} ,
\]

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 assume (55) holds and bound the second term in (26) using (56) of Theorem 8. For the \( \ell = 0 \) term in (25), we use the estimate

\[
\|G(u_{h_0}^{0})\|_{\mathcal{W}_{\gamma} \mathcal{T}} \leq \left( \sum_{u \subseteq \{1:9\}} \frac{1}{\gamma_u} \int \left( \int \frac{1}{2} \frac{1}{2} |u| \int \left( \frac{1}{2} \frac{1}{2} |u| \right) \left( \frac{1}{2} \frac{1}{2} |u| \right) \frac{1}{\gamma_u} \right) \right)^{1/2}
\]

which follows from an adaptation of (33) from Theorem 6. Combining these estimates with (22), (24), (25), (26), and (14), we obtain

\[
\mathbb{E} \left[ \frac{1}{G(u)} - G(u) \right] \leq C \left( \|f\|_{H^{-1+\varepsilon}(D)} \|G\|_{H^{-1+\varepsilon}(D)} + \theta_{\ell-1}s_{\ell-1}^{-2(1/p - 1)} \|f\|_{V^*} \|G\|_{V^*} \right)^{1/2}
\]

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 \( s_{\ell} = s_{\ell-1} \). These together with some further estimations lead to the following simplified mean-square error bound.
Theorem 9 Under Assumptions (A1)–(A6) and the condition (55) with \( n = 3 \), for every \( f \in H^{-1+\tau}(D) \) with \( 0 \leq \tau \leq 1 \) and every \( G \in H^{-1+\tau}(D) \) with \( 0 \leq \tau' \leq 1 \), the mean-square error of the multi-level QMC FE algorithm defined by (19) can be estimated as follows

\[
\mathbb{E}[|I(G(u)) - Q^L(\cdot; G(u))|^2] \leq CD \rho(\lambda) \|f\|_{H^{-1+\tau}(D)}^2 \|G\|_{H^{-1+\tau}(D)}^2 \\
\cdot \left[ \left(h_F^2 + \theta_s s_L^{-2(1/p-1)}\right)^2 + \sum_{\ell=0}^{L} |\varphi(N_\ell)|^{-1/\lambda} \left(h_F^2 + \theta_{\ell-1} s_{\ell-1}^{-\min(1/p-1,\alpha)}\right)^2 \right],
\]

where

\[
D \rho(\lambda) := \left( \sum_{|u|<\infty} \gamma^2_u |\rho(\lambda)|^{|u|} \right)^{1/\lambda} \left( \sum_{|u|<\infty} \left[\frac{||u|+3|!}{|u|!}\right]^2 \prod_{j \in u} \tilde{b}_j^2 \right) \gamma_u,
\]

with \( 0 \leq \tau := \tau + \tau' \leq 2 \), \( s_{-1} := 1 \), \( \theta_{-1} := 0 \), \( \rho(\lambda) \) as in (17), and \( \tilde{b}_j \) as in (35). In general we have \( \theta_{\ell} = 1 \) for all \( \ell = 0, \ldots, L \). If \( s_{\ell} = s_{\ell-1} \) for some \( \ell \geq 1 \) then \( \lambda_{\ell-1} = 0 \). When \( k \)-orthogonality (28) holds we have \( \theta_{\ell} = 0 \) for all \( \ell = 0, \ldots, L \). Assumptions (A3) and (A5) and the condition (55) 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 \([0,1]^n\). The error bound (61) is meaningful only if \( D \rho(\lambda) \) is finite.

3.6 Choosing the Parameter \( \lambda \) and the Weights \( \gamma_u \)

Following [24], we now choose the weights \( \gamma_u \) to minimize \( D \rho(\lambda) \). 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 (63) is implied by Assumption (A7).

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

\[
\sum_{j \geq 1} \tilde{b}_j^q < \infty \quad \text{for some} \quad 0 < q \leq 1,
\]

and when \( q = 1 \) assume additionally that

\[
\sum_{j \geq 1} \tilde{b}_j < \sqrt{6}.
\]

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

\[
\gamma_u = \gamma_u(\lambda) := \left( \frac{||u|+3|!}{6} \prod_{j \in u} \tilde{b}_j \sqrt{\rho(\lambda)} \right)^{2/(1+\lambda)}
\]

(65)
minimizes $D_q(\lambda)$ given in (62), if $D_q(\lambda) < \infty$. Moreover, the choice of $\lambda$ given by

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

(66)

together with $\gamma_u = \gamma_u(\lambda_q)$, ensures that $D_q(\lambda_q) < \infty$, and thus justifies the error bound (61).

**Proof** This proof follows closely the proof of [24, Theorem 6.4]. 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 $[|u| + 3]$ instead of $|u|$. For this we make use of [24, Lemma 6.3] with $n = 3$ instead of $n = 0$.

Using [24, Lemma 6.2], we see that $D_q(\lambda)$ is minimized by choosing $\gamma_u$ as in (65) for $|u| < \infty$, provided that $D_q(\lambda) < \infty$. We add that an overall rescaling of weights does not affect the minimization argument. Our choice of scaling here is consistent with the convention that $\gamma_q := 1$.

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 (65), we have

$$
\sum_{|u| < \infty} (\gamma_u^*)^{\lambda} |\rho(\lambda)|^{|u|} = 6^{-2\lambda/(1+\lambda)} A_\lambda, \quad \sum_{|u| < \infty} \frac{[(|u| + 3)]^2 \prod_{j \in \mathbb{Z}} \bar{b}_j^2}{\gamma_u} = 6^{2/(1+\lambda)} A_\lambda,
$$

and thus $D_q(\lambda) = A_\lambda^{1/\lambda + 1}$, where

$$
A_\lambda := \sum_{|u| < \infty} [(|u| + 3)]^{2\lambda/(1+\lambda)} \prod_{j \in \mathbb{Z}} \left( \frac{\bar{b}_j^{2\lambda} \rho(\lambda)}{\alpha_j^{2\lambda}} \right)^{1/(1+\lambda)}.
$$

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 $\prod_{j \in \mathbb{Z}} \alpha_j^{2\lambda/(1+\lambda)}$, 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

$$
A_\lambda \leq \left( \sum_{|u| < \infty} [(|u| + 3)] \prod_{j \in \mathbb{Z}} \alpha_j^{2\lambda/(1+\lambda)} \right)^{2\lambda/(1+\lambda)} \left( \sum_{|u| < \infty} \prod_{j \in \mathbb{Z}} \left( \frac{\bar{b}_j^{2\lambda} \rho(\lambda)}{\alpha_j^{2\lambda}} \right)^{1/(1+\lambda)} \right)^{(1-\lambda)/(1+\lambda)}
$$

$$
\leq \left[ 6 \left( \frac{1}{1 - \sum_{j \geq 1} \alpha_j} \right)^{2\lambda/(1+\lambda)} \right]^{2\lambda/(1+\lambda)} \exp \left( \frac{1 - \lambda}{1 + \lambda} |\rho(\lambda)|^{1/(1-\lambda)} \sum_{j \geq 1} \left( \frac{\bar{b}_j}{\alpha_j} \right)^{2\lambda/(1-\lambda)} \right).
$$
which holds and $A_k$ is finite, see [24, Lemma 6.3], provided that
\[ \sum_{j \geq 1} \alpha_j < 1 \quad \text{and} \quad \sum_{j \geq 1} \left( \frac{\bar{b}_j}{\alpha_j} \right)^{2\lambda/(1-\lambda)} < \infty. \quad (67) \]

We now choose
\[ \alpha_j := \frac{\bar{b}_j}{\sigma} \quad \text{for some parameter} \quad \sigma > \sum_{j \geq 1} \bar{b}_j. \]

Then the first sum in (67) is less than 1 due to the assumption (63). Noting that (63) implies that $\sum_{j \geq 1} \bar{b}_j < \infty$ for all $q' \geq q$, we conclude that the second sum in (67) converges for
\[ \frac{2\lambda}{1-\lambda} (1-q) \geq q \iff q \leq \frac{2\lambda}{1+\lambda} \iff \lambda \geq \frac{q}{2-q}. \]

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 $\rho(1) = 1/6$. Then using [24, Lemma 6.3] and the assumption (64) we obtain
\[ A_1 = \sum_{|u| < \infty} (|u| + 3)! \prod_{j \in u} \left( \frac{\bar{b}_j}{\sqrt{6}} \right) \leq 6 \left( \frac{1}{1 - \sum_{j \geq 1} (\bar{b}_j/\sqrt{6})} \right)^4 < \infty. \]

This completes the proof. □

In the following theorem we verify that with a slightly modified choice of weights the condition (55), which is required in Theorem 9, is indeed satisfied. The assumptions in the theorem are consistent with Assumptions (A3), (A5), and (A7), however, the requirement that $p$ be strictly smaller than $q$ is new, and is essential for obtaining the decay we need.

**Theorem 11** With $b_j$ and $\bar{b}_j$ defined as in (12) and (35) for fixed $\kappa \in (0, 1]$, suppose that the sequence $\{b_j\}$ is non-increasing and
\[ \sum_{j \geq 1} b_j^p < \infty \quad \text{and} \quad \sum_{j \geq 1} \bar{b}_j^q < \infty \quad \text{for some} \quad 0 < p < q \leq 1. \]

Define a new sequence $\{\beta_j\}$ by
\[ \beta_j := \max(\bar{b}_j, b_j^{p/q}). \]

Then, Theorems 9 and 10 hold a fortiori if $\bar{b}_j$ is replaced by $\beta_j$. Moreover, the choice of weights (65) with $\beta_j$ instead of $\bar{b}_j$ satisfies the condition (55) with $n = 3$ and
\[ \alpha = \frac{1}{p} - \frac{1}{q}. \]

However, the constant $C$ in Theorem 9 has now a dependence on $\lambda$. 


Proof} Note that \( \sum_{j \geq 1} \beta_j^q < \infty \). Substituting (65), with \( b_j \) replaced by \( \beta_j \), into the left-hand side of (55), we obtain

\[
\sum_{u \subseteq \{1:x_l\} \setminus \{x_{l-1}+1:x_l\} \neq \emptyset} (|u|!)^2 \prod_{j \in u} b_j^2 = \frac{\sum_{u \subseteq \{1:x_l\}} (|u|!)^2 \prod_{j \in u} b_j^2}{\frac{1}{|b|} (|u| + 3)! \prod_{j \in u} (b_j/\sqrt{\lambda}(\lambda)^{2/(1+\lambda)})^{2/(1+\lambda)}},
\]

where in the last step we allowed \( u \) to also include the index \( k \), and used \( \beta_k \geq \beta_k^p/q \) and \( (|u| + 1)! \geq (|u| + 3)! \) in the denominator, and \( (|u| + 1)! \leq (|u| + 3)! \) in the numerator.

To complete the proof, we estimate the tail sum \( \sum_{k \geq x_{l-1}+1} b_k^{2-2(p/q)/(1+\lambda)} \) using (14), but with \( b_j \) replaced by \( b_j^{2-2(p/q)/(1+\lambda)} \) and \( p \) replaced by \( p/[2-2(p/q)/(1+\lambda)] \). This is valid because

\[
\frac{2-2(p/q)/(1+\lambda)}{p} \geq \frac{2}{p} \frac{2}{q(1+q/(2-q))} = \frac{2}{p} - \frac{2}{q} + 1 > 1,
\]

where we used \( \lambda \geq q/(2-q) \). The exponent of \( s_{l-1} \) in (55) becomes \(-2(2/p - 2/q)\), proving that (55) holds with \( \alpha = 1/p - 1/q \), but with a constant in front that now depends on \( \lambda \).

\[\square\]

\subsection*{3.7 Summary of Overall Cost Versus Error}

Recall that

\[
h_{\ell} \asymp 2^{-\ell} \quad \text{and} \quad M_{h_{\ell}} \asymp h_{\ell}^{-d} \asymp 2^{-d\ell} \quad \text{for} \quad \ell = 0, \ldots, L. \tag{70}
\]

Based on the mean square error bound (61), 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. We assume that in general the cost for assembling the stiffness matrix at level \( \ell \) is \( \mathcal{O}(s_{\ell} M_{h_{\ell}}) \), 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 $K_r$. (Some cost models in the literature do not include $s_\ell$ as part of $K_r$.) Note that our cost model does not include the pre-computation cost for the CBC construction of randomly shifted lattice rules, which requires $O(s_\ell N\ell \log N_\ell + s_\ell^2 N_\ell)$ 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 (61), giving the mean square error bound (denoted in this subsection by error$^2$ for simplicity)

$$
\text{error}^2 = \Theta \left( h_\ell^{2\tau} + \sum_{\ell=0}^{L} \frac{1}{\gamma(N_\ell)}^{-1/2} h_{\ell-1}^{2\tau} \right).
$$

**Scenario 2.** When $k$-orthogonality (28) does not hold and $p < q \leq 1$, we have $\theta_\ell = 1$ in the error bound (61). We assume that the weights $\gamma_\ell$ are chosen as in Theorem 11, so that (69) holds. To balance the error contribution within the highest discretization level, we impose the condition $s_\ell \approx 2/(p-1) = \Theta(h_\ell^2)$, which is equivalent to $s_\ell = \Omega(2^{L\ell p/(2-2p)})$. 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 $\theta_{L-1} = 0$ for all $\ell = L, \ldots, L$ in (61). 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 $s_{\ell-1}^{-(1/p-1/q)} = \Theta(h_{\ell-1}^2)$ for $\ell = 1, \ldots, L$ (see (61) with $\alpha = 1/p - 1/q$), which is equivalent to $s_{\ell} = \Omega(2^{L\ell p/(q-p)})$ for $\ell = 0, \ldots, L-1$. Combining both approaches, while taking into account the monotonicity condition (18), we choose

$$
\begin{align*}
   s_\ell := \min \left( 2^{L\ell p/(q-p)}, 2^{L\ell p/(2-2p)} \right) & \quad \text{for} \quad \ell = 0, \ldots, L .
\end{align*}
$$

Thus we have $s_\ell$ strictly increasing for $\ell = 0, \ldots, \lfloor L(q-p)/(q(2-2p)) \rfloor$, and the remaining $s_\ell$ are all identical. This leads again to the error bound (71).

**Scenario 3.** When $k$-orthogonality (28) does not hold and $p = q < 1$, we choose

$$
\begin{align*}
   s_\ell := 2^{L\ell p/(2-2p)} & \quad \text{for} \quad \ell = 0, \ldots, L .
\end{align*}
$$

This again yields the error bound (71).

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 $1/\varphi(N) < (e^3 \log \log N + 3/\log \log N)/N$ for all $N \geq 3$, where $e^3 = 1.781 \ldots$. 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 $h_{\ell-1} \approx h_\ell$, we obtain for all three scenarios the simpler mean square error expression

$$
\text{error}^2 = \Theta \left( h_\ell^{2\tau} + \sum_{\ell=0}^{L} N_\ell^{-1/2} h_{\ell-1}^{2\tau} \right).
$$
To minimize the mean square error for a fixed cost, we consider the Lagrange multiplier function

$$g(\mu) := h_L^{2\tau} + \sum_{\ell=0}^{L} N_{\ell}^{-1/\lambda} h_{\ell}^{2\tau} + \mu \sum_{\ell=0}^{L} N_{\ell} K_{\ell}.$$

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

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

This prompts us to define

$$N_{\ell} := \left[ N_{0} \left( h_{0}^{-2\tau} K_{0} h_{0}^{2\tau} K_{0}^{-1} \right)^{\lambda/(\lambda + 1)} \right] \quad \text{for} \quad \ell = 1, \ldots, L. \quad (74)$$

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

$$\text{error}^2 = \mathcal{O}\left( h_L^{2\tau} + N_0^{-1/\lambda} \sum_{\ell=0}^{L} E_\ell \right) \quad \text{and} \quad \text{cost} = \mathcal{O}\left( N_0 \sum_{\ell=0}^{L} E_\ell \right), \quad (75)$$

where

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

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 $\ell$) decreases with increasing $\ell$.
- For $d > 2\lambda \tau$, the quantity $E_{\ell}$ increases with increasing $\ell$.

In the light of the error bound in (75), we always choose $N_0$ to satisfy

$$N_0^{-1/\lambda} \sum_{\ell=0}^{L} E_\ell = \mathcal{O}\left( h_L^{2\tau} \right) \iff N_0 = \Omega\left( h_L^{-2\tau \lambda} \left( \sum_{\ell=0}^{L} E_\ell \right)^{\lambda} \right), \quad (76)$$

leading to the simplified error bound $\text{error}^2 = \mathcal{O}\left( h_L^{2\tau} \right)$.

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

$$\sum_{\ell=0}^{L} E_{\ell} = \mathcal{O}\left( \sum_{\ell=0}^{L} 2^{-\ell(2\lambda \tau - d)/(\lambda + 1)} (\ell + 1)^{1/(\lambda + 1)} \right)$$

$$= \begin{cases} \mathcal{O}\left( \left(1\right) \right) & \text{if } d < 2\lambda \tau, \\ \mathcal{O}\left( \left(L^{(\lambda + 2)/(\lambda + 1)} \right) \right) & \text{if } d = 2\lambda \tau, \\ \mathcal{O}\left( \left(2^{-L(2\lambda \tau - d)/(\lambda + 1) - 1/(\lambda + 1)} \right) \right) & \text{if } d > 2\lambda \tau. \end{cases}$$
The choice \((76)\) for \(N_0\) then yields

\[
N_0 := \begin{cases} 
2L_r(2\lambda) & \text{if } d < 2\tau\lambda, \\
2L_r(2\lambda)\frac{\lambda}{\lambda+1} & \text{if } d = 2\tau\lambda, \\
2L_r(d+\tau\lambda)\frac{\lambda}{\lambda+1} & \text{if } d > 2\tau\lambda.
\end{cases}
\]  

(77)

Upon substituting \((76)\) into the cost bound in \((75)\) and using \((77)\), we obtain

\[
\text{cost} = \mathcal{O}\left(N_0^{\lambda+1/\lambda} h^2 \tau\right) = \begin{cases} 
\mathcal{O}\left(2L_r(2\lambda)\right) & \text{if } d < 2\lambda\tau, \\
\mathcal{O}\left(2L_r(2\lambda)\frac{\lambda}{\lambda+1}\right) & \text{if } d = 2\lambda\tau, \\
\mathcal{O}\left(2L_r(d+\tau\lambda)\frac{\lambda}{\lambda+1}\right) & \text{if } d > 2\lambda\tau.
\end{cases}
\]

Scenario 2 (continued). When \(k\)-orthogonality does not hold and \(p < q \leq 1\), we use the definition \((72)\) for \(s_t\). We consider separately the two alternative choices in \((72)\):
choice A takes \(s_t = \lceil 2^{\ell} \xi \rceil\) for all \(\ell\), while choice B takes \(s_t = \lceil 2^{\ell+1} \xi \rceil\) for all \(\ell\), where

for ease of notation we have introduced

\[
\eta := \frac{pq}{q-p} \quad \text{and} \quad \xi := \frac{p}{2-2p}.
\]

(78)

noting that \(\eta \geq \xi\). Then we have \(\sum_{\ell=0}^{L} E_\ell \leq \min\left(\sum_{\ell=0}^{L} E_\ell^{(A)}, \sum_{\ell=0}^{L} E_\ell^{(B)}\right)\), where

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

(79)

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

(80)

For the “middle case” \(2\lambda - \eta < d/\tau < 2\lambda\), it is beneficial to estimate directly

\[
\sum_{\ell=0}^{L} E_\ell = \mathcal{O}\left(\sum_{\ell=0}^{L} 2^{(\ell+1)(d/\tau-2\lambda-\eta)/(\lambda+1)} + 2L_r\xi/(\lambda+1) \sum_{\ell=\lceil 2L_r\xi/(\lambda+1) \rceil}^{L} 2^{(\ell+1)(d/\tau-2\lambda)/(\lambda+1)}\right) = \mathcal{O}\left(2L_r\xi/(\lambda+1)\right).
\]

(81)
Comparing this with (79) and (80), and taking the appropriate minimum, we obtain

\[
\sum_{t=0}^L E_t = \begin{cases}
\mathcal{O}(1) & \text{if } d/\tau < 2\lambda - \eta, \\
\mathcal{O}(L) & \text{if } d/\tau = 2\lambda - \eta, \\
\mathcal{O}(2^{Lt}(\xi/\eta)(d/\tau - 2\lambda + \eta)/(\lambda + 1)) & \text{if } 2\lambda - \eta < d/\tau < 2\lambda, \\
\mathcal{O}(2^{Lt+\xi/(\lambda+1)\lambda}) & \text{if } d/\tau = 2\lambda, \\
\mathcal{O}(2^{Lt}(d/\tau - 2\lambda + \xi)/(\lambda + 1)) & \text{if } d/\tau > 2\lambda.
\end{cases}
\]

The choice (76) for \( N_0 \) yields

\[
N_0 := \begin{cases}
[2^{Lt}(2\lambda)] & \text{if } d/\tau < 2\lambda - \eta, \\
[2^{Lt}(2\lambda) L^\lambda] & \text{if } d/\tau = 2\lambda - \eta, \\
[2^{Lt}(2\lambda + 1)(\xi/\eta)(d/\tau - 2\lambda + \eta)/(\lambda + 1)] & \text{if } 2\lambda - \eta < d/\tau < 2\lambda, \\
[2^{Lt}(2\lambda + 1)(\xi)/(\lambda + 1)L^\lambda] & \text{if } d/\tau = 2\lambda, \\
[2^{Lt+\xi/(\lambda+1)\lambda}] & \text{if } d/\tau > 2\lambda.
\end{cases}
\]

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

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

Scenario 3 (continued). When k-orthogonality (28) does not hold and \( p = q < 1 \), we proceed in a similar way, taking \( s_t = [2^{Lt+\xi}] \) with \( \xi \) given by (78), to obtain

\[
N_0 := \begin{cases}
[2^{Lt}(2\lambda + 1)(\xi)/(\lambda + 1)] & \text{if } d/\tau < 2\lambda, \\
[2^{Lt}(2\lambda + 1)(\xi)/(\lambda + 1)L^\lambda] & \text{if } d/\tau = 2\lambda, \\
[2^{Lt+\xi/(\lambda+1)\lambda}] & \text{if } d/\tau > 2\lambda.
\end{cases}
\]

and

\[
\text{cost} = \begin{cases}
\mathcal{O}(2^{Lt}(2\lambda + \xi)) & \text{if } d/\tau < 2\lambda, \\
\mathcal{O}(2^{Lt}(2\lambda + \xi)L^\lambda) & \text{if } d/\tau = 2\lambda, \\
\mathcal{O}(2^{Lt}(d/\tau + \xi)) & \text{if } d/\tau > 2\lambda.
\end{cases}
\]

In all three scenarios, for given \( \epsilon > 0 \), we choose \( L \) such that

\[
h_L^{2\tau} \approx 2^{-L\tau} \approx \epsilon.
\]

We can then express the total cost of the algorithm in terms of \( \epsilon \). This is summarized in Theorem 12 below.
Theorem 12 Under Assumptions (A1)–(A7), leaving out (A5) if k-orthogonality (28) holds, for \( f \in H^{-1+t}(D) \) and \( G \in H^{-1+t'}(D) \) with \( 0 \leq t, t' \leq 1 \) and \( \tau := t + t' > 0 \), consider the multi-level QMC FE algorithm defined by (19). Given \( \varepsilon > 0 \), with \( L \) given by (83), \( h_\ell \) given by (70), \( s_\ell \) given by (29), (72) or (73) as appropriate, \( N_\ell \) given by (74), \( N_p \) given by (77), (81) or (82) as appropriate, and with randomly shifted lattice rules constructed based on POD weights \( \gamma_0 \) given by (65), in which \( \beta_j \) is replaced by \( \beta_\ell \) from (68), we obtain

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

and

\[
\text{cost}(Q_\ell^L) = \mathcal{O}(\varepsilon^{-\lambda_{\text{ML}}}(\log \varepsilon^{-1})^{b_{\text{ML}}}),
\]

with

\[
a_{\text{ML}} = \begin{cases} 
2\lambda_q \frac{d}{\tau} & \text{if k-orthogonality (28) holds,} \\
\max \left( 2\lambda_q \frac{d}{\tau}, \frac{p}{2} - 2p \left( 1 - \frac{q - p}{pq} \frac{d}{\tau} \right) \right) & \text{otherwise}.
\end{cases}
\]

where \( \lambda_q \) is as defined in (66). 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 [24] 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 [24, Theorem 8.1], where \( \lambda_p \) is defined analogously to \( \lambda_q \) as follows

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

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 \( a_{\text{ML}}^{83} = 2 \) under k-orthogonality. In a number of examples it can be shown that \( q \leq 1 \) implies \( p \leq 1/2 \), which is stronger than just \( p \leq 1 \) as required in the single level algorithm.

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, 36], 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 [27] 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 is 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 \(yy_y\) and in the smoothness scale \(Z\) with respect to the spatial variable \(xx_x\)).

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 \(O(h_L)\) in the norm of \(V\) (rather than for linear functionals of the solution) can be computed in \(O(M_h) = O(h_L^{-2})\) 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 [24], 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 probability model in these papers, namely, independent and uniformly distributed parameters \(y_j\), is particularly simple and lends itself naturally to an error analysis by QMC. The aim of the present multi-level version of the QMC approach is to outline the design of a multilevel QMC FE 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 [24]) 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 \(l = l' = 1\) 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 \(O((2^{2L} / (1 - \delta))) = O(h_L^{-2(1 - \delta)})\), while the convergence rate is the (best possible) second order \(O(2^{-2L}) = O(h_L^{-2})\). 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 \(a(x,y)\), 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 $G \in L^2(D)$, ensure in (6) that $Z = (H_0^1 \cap H^2)(D)$ and, in turn, implies $O(h^2)$ convergence in (16). The present convergence analysis extends directly to weaker assumptions: if in (A4) and (A7) we have only Hölder continuity $C^{0,r}(\overline{D})$ for some $0 < r < 1$ instead of $W^{1,\infty}(D)$ regularity, or if $D$ is not convex, then $\tilde{b}_j$ in (35) and (65) will depend on $\|\psi_j\|_{C^{0,r}(\overline{D})}$ 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 $y$, but Theorem 6 holds for higher order mixed derivatives. The results here can be extended by considering higher order QMC methods, see e.g. [11, Chapter 15].

Finally, in our multi-level scheme we assumed that exact expectations $E[\cdot]$ over all realizations of random shifts $\Delta_j \in [0,1]^d$ 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 $\Delta_j$, at discretization level $\ell = 0,1,...,L$. This leads to a further error $(E - E_{m\ell})[\cdot]$ in term $\ell$ of (23) of order $O(m^{-1})$. 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 $\Delta_j$ for each level $\ell$. To provide a reasonable error estimate, our experience (stemming, in part, from Monte-Carlo simulations) is that the number $m^*$ of realizations of random shifts needs to be of the order of 10 to 30.

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