Multilevel Sparse Grid Methods for Elliptic Partial Differential Equations with Random Coefficients

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Abstract

Stochastic sampling methods are arguably the most direct and least intrusive means of incorporating parametric uncertainty into numerical simulations of partial differential equations with random inputs. However, to achieve an overall error that is within a desired tolerance, a large number of sample simulations may be required (to control the sampling error), each of which may need to be run at high levels of spatial fidelity (to control the spatial error). Multilevel sampling methods aim to achieve the same accuracy as traditional sampling methods, but at a reduced computational cost, through the use of a hierarchy of spatial discretization models. Multilevel algorithms coordinate the number of samples needed at each discretization level by minimizing the computational cost, subject to a given error tolerance. They can be applied to a variety of sampling schemes, exploit nesting when available, can be implemented in parallel and can be used to inform adaptive spatial refinement strategies. We extend the multilevel sampling algorithm to sparse grid stochastic collocation methods, discuss its numerical implementation and demonstrate its efficiency both theoretically and by means of numerical examples.

Keywords: uncertainty quantification, multilevel sampling, sparse grid sampling, elliptic partial differential equations

1. Introduction

Computing has become an invaluable tool in modern science and engineering because, increasingly, computer simulations are used to supplement or replace experiments and prototype engineering systems, and to predict the behavior of complex physical processes. Often, however, the precise environmental conditions (or model parameters) surrounding the process that is being simulated are known only with a limited degree of certainty. For systems governed by partial differential equations (PDEs) with random inputs, statistical sampling methods present arguably the most direct and least intrusive means of incorporating parametric uncertainty into numerical simulations. Descriptive statistics related to the random simulation output are obtained by generating representative samples of the input parameters and then running the numerical simulation for each sample point, yielding sample of outputs that can then be aggregated statistically.

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To be more specific, let \((\Omega, \mathcal{F}, \mathbb{P})\) denote the complete probability space underlying the system’s uncertain input parameters. For any sample point \(\omega \in \Omega\) corresponding to a given system configuration, let \(u(x, \omega)\) denote the resulting simulation output and let \(G_1(u(x, \omega))\) denote a physical output of interest (e.g., a function value, a spatial average, the total energy, or the flux across a boundary) that is determined from \(u(x, \omega)\). A large class of statistical quantities of interest \(Q\) associated with an output of interest \(G_1(u(x, \omega))\) take the form of a stochastic integral or expectation, i.e.,

\[
Q := \mathbb{E}[G_2(G_1(u))] = \int_{\Omega} G_2(G_1(u(x, \omega))) \, d\mathbb{P}(\omega) \tag{1}
\]

for an appropriate choice of \(G_2\); for example, if \(G_2(v) = v^k\), then \(Q\) is the \(k\)th raw statistical moment of \(G_1(u)\) or, if \(G_2(v) = \chi\{G_1(u) \geq a\}\), where \(\chi\) is the characteristic function, then \(Q\) equals the exceedance probability \(\mathbb{P}[G_1(u(\omega)) \geq a]\). Because this paper addresses the numerical approximation of the integral (1), it is not essential for us to know the details about how the integrand is constructed from the output of interest \(G_1\) and the desired statistical information embodied in \(G_2\). Thus, we can refer directly to the integrand by letting \(G = G_2 \circ G_1\) so that we rewrite (1) as

\[
Q = \mathbb{E}[G(u)] = \int_{\Omega} G(u(x, \omega)) \, d\mathbb{P}(\omega). \tag{2}
\]

In general, input functions that are modeled as spatially varying random fields are first approximated by functions of a finite-dimensional random parameter vector \(\vec{y}(\omega) := (y_1(\omega), \ldots, y_N(\omega))\) with range in some hyper-rectangle \(\Gamma = \prod_{n=1}^{N} \Gamma_n \subset \mathbb{R}^N\) and known joint probability density function \(\rho : \Gamma \rightarrow [0, \infty)\). Such “finite noise” approximations may be achieved through an expansion in terms of piecewise constant functions based on a subdivision of the spatial domain, or through truncated spectral expansions related to the field’s correlation function, e.g., via Karhunen-Loève expansions; see [1, 2, 3]. Under this approximation, the statistical quantity of interest \(Q\) given by (2) takes the form of a high-dimensional integral, i.e.,

\[
Q = \mathbb{E}[G(u)] = \int_{\Gamma} G(u(x, \vec{y})) \rho(\vec{y}) \, d\vec{y}, \tag{3}
\]

where \(\vec{y}\) denotes the vector of random parameters.

In practice, for any \(\vec{y} \in \Gamma\), only spatial approximations \(u_h(x, \vec{y})\) (determined via, e.g., finite element, finite difference, finite volume, or spectral methods) of the solution \(u(x, y)\) are available. Here \(h\) is a spatial discretization parameter that is often related to the spatial grid size. As a result, instead of (3), one can only determine the approximation

\[
Q \approx Q_h := \mathbb{E}[G(u_h)] = \int_{\Gamma} G(u_h(x, \vec{y})) \rho(\vec{y}) \, d\vec{y} \tag{4}
\]

of the quantity of interest \(Q\).

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1Of course, the simulation output could also depend on time, but for the sake of simplicity, we suppress mention of such possible dependences.
A statistical sampling method is simply a numerical quadrature scheme that estimates the statistical quantity of interest given by (3) or (4) by a quadrature rule, e.g., in the latter case, a weighted sum of the form

\[ Q \approx Q_{M,h} := \sum_{m=1}^{M} \mu_m G(u_h(x, \gamma^m)), \]  

(5)

where \( \{\gamma^m\}_{m=1}^{M} \) denotes a collection of samples of \( \gamma \in \Gamma \) and \( \{\mu_m\}_{m=1}^{N} \) a given set of weights. Note the evaluation of \( Q_{M,h} \) requires \( M \) solutions \( \{u_h(x, \gamma^m)\}_{m=1}^{M} \) of the discretized PDE, one for each of the \( M \) samples \( \gamma^m \) of the parameter vector \( \gamma \). Depending on the statistical complexity of the underlying parametric uncertainty and on the sampling scheme used, an accurate approximation \( Q_{M,h} \) of \( Q \) may require a large number of simulation runs, i.e., \( M \) may be large; clearly, this can be computationally intensive, especially when individual simulations are run at a high level of spatial fidelity, i.e., for small \( h \). Increasing \( N \), i.e., increasing the dimension of the parameter space, especially results in explosive growth in computational complexity, a phenomena commonly referred as the \textit{curse of dimensionality}.

Monte Carlo (MC) sampling provides a straightforward means of approximating the integral in (3) by generating \( M \) random samples \( \gamma^m \in \Gamma, m = 1, \ldots, M \), based on the PDF \( \rho(\gamma) \) and then simply averaging the resulting \( G(u_h(x, \gamma^m)) \). Thus, \( \mu_m = 1/M \) for all \( m \) and (5) becomes

\[ Q \approx Q_{MC, h} = \frac{1}{M} \sum_{m=1}^{M} G(u_h(x, \gamma^m)). \]  

(6)

Although the MC method is largely immune from the curse or dimensionality, its suffers from very slow convergence with respect to increasing \( M \). In fact, the rate at which the root mean squared error converges is \( O(M^{-1/2}) \). This has motivated the development of multilevel Monte Carlo (MLMC) methods. These methods aim to achieve the same accuracy as traditional MC methods but at a reduced computational cost by making use of a hierarchy of spatial simulation models having increasing fidelity, e.g., based on decreasing values of \( h \). The MC method as described by (6) uses a single spatial model, i.e., a single value of \( h \). MLMC methods were first introduced in [4] for the evaluation of parametric integrals, especially those arising from the approximation of integral equations. In [5, 6, 7], the algorithm is further developed, extending its application to numerical simulations of stochastic differential equations related to computational finance. In [8], a version of the method was adapted to finite element approximations of elliptic partial differential equations with stochastic inputs. There, the sample sizes were chosen to equilibrate the sampling and spatial discretization errors at each refinement level, resulting in approximations of \( Q \) that, in certain cases, are of log-linear complexity. This approach was generalized to include a variety of other stochastic sampling schemes in [9], where its behavior was explained through analogies with sparse-grid methods [10].

In [11], an altogether more conceptual view was taken by examining the MLMC method as a numerical optimization problem. The number of parameter samples needed at each spatial discretization level are coordinated so as to minimize the total computational cost, subject to a given error tolerance. Simulations based on smaller values of \( h \) are sampled sparingly, whereas those based on coarser grids form the bulk of the sampling, where possible. This framework lends a certain degree of flexibility to the MLMC method by allowing for the incorporation of different spatial error estimates and statistical quantities of interest [12, 13] as well as other
factors that may influence the convergence rate such as the truncation level of the Karhunen-Loève expansion, parallel implementations, and quadrature nesting.

An alternative to sampling methods such as MC or quasi-MC methods for approximating the quantity of interest $Q$ are provided by interpolatory methods which are often referred to as stochastic collocation (SC) methods. In this setting, the parameter dependence of the spatial approximation $u_h(x, \tilde{y})$ is itself approximated in a finite dimensional space $V_M(\Gamma)$ which is spanned by a set of interpolatory basis functions $\{\psi_m\}_{m=1}^M$ that correspond to a predetermined, i.e., deterministic, set of sample points $\{\mathbf{y}_m\}_{m=1}^M$ in $\Gamma$. The basis usually consists of global fundamental Lagrange interpolating polynomials [14, 15, 16, 17]. Then, in this case, the full approximation of $u(x, \tilde{y})$ with respect to both the spatial variable $x$ and parameter vector $\tilde{y}$ takes the form of the interpolant

$$u(x, \tilde{y}) \approx I_M u_h(x, \tilde{y}) := \sum_{m=1}^M u_h(x, \mathbf{y}_m) \psi_m(\tilde{y}) \in V_M(\Gamma) \otimes W_h(D),$$

where $W_h(D)$ denotes, e.g., the finite-dimensional finite element space used for spatial approximation and $u_h(x, \mathbf{y}_m)$ denotes the solution of the discretized PDE for the sample parameter vector $\mathbf{y}_m$. Here, we approximate the quantity of interest $Q$ given in (5) by the quantity

$$Q \approx Q_{SC}^{M, h} := \int_{\Gamma} G(I_M u_h) \rho(\mathbf{y}) d\mathbf{y}.$$  \hfill (7)

In practice, this integral has to be further approximated. If the mapping $G(I_M u_h) : \Gamma \rightarrow \widetilde{W}(D)$ is sufficiently smooth, one can use an interpolatory quadrature rule for which the quadrature points $\{\mathbf{y}_m\}_{m=1}^M$ and Lagrange fundamental polynomial basis functions $\{\psi_m\}_{m=1}^M$ are the same as those used to define the interpolant $I_M u_h$. If $\{\mu_m\}_{m=1}^M$ denotes the corresponding quadrature weights, we then have from (7) that

$$Q_{SC}^{M, h} \approx \sum_{m=1}^M \mu_m G(I_M u_h(x, \mathbf{y}_m)) = \sum_{m=1}^M \mu_m G \left( \sum_{m=1}^M u_h(x, \mathbf{y}_m) \psi_m(\mathbf{y}_m) \right) = \sum_{m=1}^M \mu_m G(u_h(x, \mathbf{y}_m)),$$

since the Lagrange fundamental polynomials satisfy $\psi_m(\mathbf{y}_m) = \delta_{mm}$. In general, the numerical approximation of the integral in (7) can also be achieved using a different quadrature rule. The overall computational cost of this rule, however, is negligible compared to the cost of constructing the interpolant $I_M u_h$.

Thus, comparing with (5), we see that SC methods for approximating the quantity of interest are sampling methods much in the same vein as are MC methods. For the former, the sample points $\{\mathbf{y}_m\}_{m=1}^M$ and weights $\{\mu_m\}_{m=1}^M$ in (5) are chosen from an interpolatory quadrature rule whereas for the latter, they are chosen at random and with weights $1/M$ for all $m$. For both, the total computational effort is dominated by the computation of solutions of the discretized PDE at the sample points $\mathbf{y}_m$.

In this paper, in the same way as for MLMC methods [11, 12, 13], we consider reducing the cost of determining approximations of quantities using a hierarchy of spatial grids but, instead of

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2 Instead of the Lagrange fundamental polynomials, one can choose other bases such as those composed of piecewise polynomial splines [18].
using MC approximations with respect to the random parameters \( \vec{y} \), we use sparse-grid stochastic collocation methods \([14, 15, 16, 17]\). These sampling methods, based on nodal interpolation at sparse-grid points in \( \Gamma \), have been shown to yield considerably higher rates of convergence than Monte Carlo methods for integrands \( G(\vec{u}(\vec{y})) \) that depend smoothly on the random vector \( \vec{y} \in \Gamma \) and for a moderately high parameter dimension \( N \). Thus, our goal is to use a hierarchy of spatial grids to accelerate the convergence of stochastic collocation approximations \( \mathcal{Q}_{Hh}^{SC} \) defined in \( [7] \), i.e., we want to do for stochastic collocation methods what MLMC methods do for MC methods.

In Section 2, we establish the notation and describe the problem setting used throughout the paper. In Section 3, the \( \epsilon \)-cost for sparse grid stochastic collocation methods, a measure of the efficiency of a sampling scheme, is discussed as is its computation based on a priori error estimates. We introduce multilevel methods in Section 4 and derive formulae for the optimal sample size at each spatial discretization level from the error estimates given in Section 3. We also derive a theoretical bound on the \( \epsilon \)-cost that improves upon that of traditional collocation methods. Here it is necessary to distinguish between collocation methods with sampling errors with algebraic convergence, i.e., of order \( O(M^{-\mu \epsilon}) \), and those with sub-algebraic convergence, i.e., of order \( O(M^{-\mu \epsilon} \log(M)^{\mu \epsilon}) \). Current practice in multilevel algorithms is to choose the hierarchy of spatial discretizations based on a fixed, predetermined mesh refinement strategy. Numerical examples are provided in Section 5 to complement and illustrate the theoretical results.

2. Notation and Setting

In this section, we introduce notation, establish estimates for the approximation error in \( [7] \), and make assumptions that allow us to analyze the multilevel sparse grid method. Although the multilevel framework is applicable to a variety of physical models, we use the elliptic partial differential equation throughout as an illustrative example. Not only is it the most well-understood model problem in the context of sparse grid stochastic collocation methods, but it has also been used extensively as an application for multilevel Monte Carlo methods, thus serving as a useful model problem in the context of sparse grid stochastic collocation methods, but it has also been used extensively as an application for multilevel Monte Carlo methods, thus serving as a useful model problem in the context of sparse grid stochastic collocation methods.

The stationary elliptic equation with homogeneous Dirichlet boundary conditions, \( \Delta u + \rho(x) = f \) in \( \Omega \) and \( u = 0 \) on \( \partial \Omega \), is
\[
\nabla \cdot (\alpha(x, \vec{y}) \nabla u(x, \vec{y})) = f(x, \vec{y}) \quad \text{in} \quad \Omega \times \Gamma
\]
\[
u(x, \vec{y}) = 0 \quad \text{on} \quad \partial \Omega \times \Gamma.
\] (8)

with corresponding weak form: find \( u : \Gamma \rightarrow H^1_0(\Omega) \) so that
\[
\int_\Omega a(\vec{y}) \nabla u \cdot \nabla w \, dx = \int_\Omega f(\vec{y}) w \, dx \quad \forall w \in H^1_0(\Omega), \vec{y} \in \Gamma.
\] (9)

Under the assumption that \( f \in L^q_0(\Gamma; L^2(\Omega)) \) and \( a \in L^\infty(\Gamma, C^1(\Omega)) \) so that
\[
0 < a_{\min} \leq a(x, \vec{y}) \quad \text{a.s. on} \quad \Gamma \times \Omega
\]
for constant \( a_{\min} > 0 \), the solution to (9) exists, is unique and has sample paths \( u(\vec{y}) \in H^1_0(\Omega) \cap H^2(\Omega) \). In fact, there exists a constant \( C_{\text{reg}} > 0 \) independent of \( \vec{y} \) so that \( ||u(\vec{y})||_{H^1} \leq C_{\text{reg}} ||f(\vec{y})||_{L^2} \)
for all \( \tilde{y} \in \Gamma \) and hence \( u \in L^\infty_p(\Gamma, H^1_0(D) \cap H^2(D)) \).

Our goal is to derive an estimate for \( \|Q - Q_{M,h}\|_W \). It is convenient to use the linearity of the expectation, together with the triangle inequality to split the total error into a spatial discretization error and a sampling error, i.e.

\[
\|Q - Q_{M,h}\|_W \leq \|Q - Q_b\|_W + \|Q_b - Q_{M,h}\|_W,
\]

(10)

where \( \| \cdot \|_W \) is the norm on \( \tilde{W}(D) \). Here, the spatial discretization error is independent of the sampling error and can thus be considered separately.

2.1. Spatial discretization error

We estimate the first term of the right-hand side of (10). With regards to the output of interest \( G(u) \), we make the following assumptions.

**Assumption 1.** (i) For each \( \tilde{y} \in \Gamma \), \( u(x, \tilde{y}) \in W(D) \) and \( G(u(x, \tilde{y})) \in \tilde{W}(D) \) for appropriate function spaces \( W(D) \) and \( \tilde{W}(D) \). For second-order elliptic problems, often \( W(D) = H^1(D) \) or a subspace of that Sobolev space; if \( G(u) \) is a functional, then \( \tilde{W}(D) = \mathbb{R} \).

(ii) For all \( u_1(x, \tilde{y}), u_2(x, \tilde{y}) \in W(D) \) and \( \tilde{y} \in \Gamma \), the mapping \( G : W(D) \rightarrow \tilde{W}(D) \) satisfies the Lipschitz condition

\[
\|G(u_1(\cdot, \tilde{y})) - G(u_2(\cdot, \tilde{y}))\|_W \leq C_G(\tilde{y})\|u_1(\cdot, \tilde{y}) - u_2(\cdot, \tilde{y})\|_W,
\]

(11)

where the Lipschitz constant \( C_G(\tilde{y}) \in L^1(\Gamma) \).

The regularity assumption (11) together with the Jensen and Hölder inequalities yield that

\[
\|Q - Q_b\|_W = \|\mathbb{E}[G(u) - G(u_b)]\|_W \leq \mathbb{E}[\|G(u) - G(u_b)\|_W] \\
\leq \mathbb{E} [C_G]\|u - u_b\|_W \leq \mathbb{E} [C_G]\|u - u_b\|_{L^2(\Gamma, W)}.
\]

(12)

The spatial error \( \|u - u_b\|_{L^2(\Gamma, W)} \) can often be approximated by means of traditional finite element analyses; see, e.g., [19]. For second-order elliptic PDEs with homogeneous Dirichlet boundary conditions, under standard assumptions on the spatial domain \( D \) and the data, one can choose \( W(D) = H^s(D) \), \( s = 0 \) or 1, i.e., we can measure the error in either the \( H^s(D) \) or \( H^0(D) = L^2(D) \) norms. One can then construct \( u_b(x, \tilde{y}) \in V_h(D) \subset H^s_0(D) \), where \( V_h(D) \) denotes a standard finite element space of continuous piecewise polynomials of degree at most \( r \) based on a regular triangulation \( T_h \) of the spatial domain \( D \) with maximum mesh spacing parameter \( h := \max_{r \in T_h} \text{diam}(r) \). We then have the error estimate [19]

\[
\|u(\cdot, \tilde{y}) - u_b(\cdot, \tilde{y})\|_{H^s(D)} \leq c h^{s+1-\gamma} \|u(\cdot, \tilde{y})\|_{H^{r-\gamma}(D)} \quad \text{for } s = 0, 1 \text{ and for a.e. } \tilde{y} \in \Gamma,
\]

(13)

where \( c > 0 \) is independent of \( \tilde{y} \) and \( h \). Hence,

\[
\|u - u_b\|_{L^2(\Gamma, H^s(D))} \leq c h^{s+1-\gamma} \|u\|_{L^2(\Gamma, H^{r-\gamma}(D))} \quad \text{for } s = 0, 1.
\]

(14)

For finite element error estimates under less rigid conditions, see, e.g., [12, 20]. Combining (12) and (13) yields

\[
\|\mathbb{E}[G(u) - G(u_b)]\|_W \leq c h^{s+1-\gamma} \|C_G\|_{L^1(\Gamma)} \|u\|_{L^2(\Gamma, H^{r-\gamma}(D))}.
\]

(15)
2.2. Sampling Error

In light of Assumption 1, the sampling error in (10) can be bounded as follows

\[
\|Q_h - \overline{Q}_h\|_{W^p} = \|E[G(u_h) - G(I_M u_h)]\|_{W^p} \leq E[\|G(u_h) - G(I_M u_h)\|_{W^p}]
\]

\[
\leq \|C_G\|_{L^2} \|u_h - I_M u_h\|_{L^2} = \Gamma(c,w)
\]

It therefore suffices to consider only the error of interpolating finite element solutions \(u_h\) in the stochastic variable \(\vec{y} \in \Gamma\). In the following, we briefly outline the construction of sparse grid interpolants and elaborate on the resulting interpolation error estimates that we will make use of in the following sections.

Most \(N\)-dimensional interpolants are constructed through some combination of lower dimensional interpolants. For each component \(\Gamma_n \subset \mathbb{R}\) of \(\Gamma\), let

\[
V_{\nu}(\Gamma;W(D)) = \left\{ \sum_{j=1}^{m_n} c_j \psi^i_n : c_j \in W(D) \text{ for } j = 1, \ldots, m_n \right\},
\]

where \(\psi^1_n, \ldots, \psi^{m_n}_n\) is a set of one-dimensional nodal basis functions with interpolation level \(i_n\) and based on \(m_n\) nodal points \(y^1_n, \ldots, y^{m_n}_n\). Furthermore, define \(\mathcal{V}^\nu : C^0(\Gamma_n; W(D)) \to V_{\nu}(\Gamma_n; W(D))\) to be the one-dimensional interpolation operator on \(\Gamma_n\), so that for any one-dimensional function \(u\) and any point \(y_n \in \Gamma_n\),

\[
\mathcal{V}^\nu(u)(y_n) = \sum_{j=1}^{m_n} u(y_n^i_n) \psi^i_n(y_n).
\]

The full tensor product interpolant of level \(\nu\) approximates an \(N\)-dimensional function \(u : \Gamma \to W(D)\) by the product of one-dimensional interpolants, each with interpolation level \(i_n = \nu\), i.e.

\[
u(y) \approx \mathcal{V}^\nu \otimes \cdots \otimes \mathcal{V}^\nu(u)(\vec{y}) := \sum_{j_1=1}^{\nu} \cdots \sum_{j_N=1}^{\nu} u(y^{j_1}_1, \ldots, y^{j_N}_N) \prod_{n=1}^{N} \psi^i_n(y_n).
\]

Computing this interpolant requires the evaluation of \(\nu\) at \(M = \prod_{n=1}^{N} m_n = (m_n)^N\) sample points, leading to a prohibitively high cost at high values of \(N\), especially if each function evaluation involves a PDE solve.

The isotropic Smolyak formula [21] constructs a multi-dimensional interpolant \(I_M u\) on \(\Gamma\) from univariate interpolants, based on a greatly reduced set of sample points \(\{y^{0}, \ldots, y^{M}\}\) while maintaining an overall accuracy not much lower than that of the full tensor product rule (see [22]). For any multi-index \(i = (i_1, \ldots, i_N) \in \mathbb{N}^N\), take \(i_n \geq 1\) to mean \(i_n \geq 1\) for \(n = 1, \ldots, N\) and let \(|i| := i_1 + \ldots + i_N\). Also for any coordinate \(y_n\) of \(\vec{y} \in \Gamma\), we write \(\vec{y} = (\vec{y}_n, y_{\nu}^n)\), where \(y_{\nu}^n \in \prod_{\nu' \neq \nu} \Gamma_{\nu'}\) are the remaining coordinates. While not computed as such, the Smolyak interpolation operator \(I_M\) of level \(\nu\) can be written as the linear combination of tensor product rules

\[
I_M = \sum_{\nu - N+1 \leq |i| \leq \nu} (-1)^{|i|} {N-1 \choose \nu + |i|} \mathcal{V}^i_0 \otimes \cdots \otimes \mathcal{V}^i_0.
\]
In the following, we restrict our attention to bounded hyper-rectangles $\Gamma$, assuming without loss of generality that $\Gamma = [-1,1]^N$, and consider the isotropic Smolyak formula based on one-dimensional Clenshaw-Curtis nodes

$$y_{j} = -\cos\left(\frac{\pi(j-1)}{m_i - 1}\right), \text{ for } j = 1, 2, \ldots, m_i,$$

with $m_i$ chosen so that

$$m_i = \begin{cases} 1, & \text{if } i = 1 \\ 2^{i-1} + 1, & \text{if } i > 1 \end{cases}$$

to ensure nestedness. Extensions of the Smolyak formula to unbounded domains with non-nested Gaussian abscissas can be found in [16], while [17] discusses anisotropic Smolyak formulae in which coordinate directions can be weighted differently, according to their relative importance.

For the purposes of error estimation for sparse grid methods, the integrand $u_h$ is often required to have bounded mixed derivatives of order $k \in \mathbb{N}_0$, i.e. to belong to the space

$$C_{\text{mix}}^k(\Gamma, W(D)) = \left\{ w : \Gamma \rightarrow W(D) : ||w||_{\text{mix},k} := \max_{\gamma \in \Gamma, r \leq k} ||D^r w(y)||_W < \infty \right\},$$

where $s = (s_1, \ldots, s_N)$ is a multi-index in $\mathbb{N}_0^N$.

Conditions on the smoothness of the model output $u_h$ in $\vec{y} \in \Gamma$ depend on the underlying physical model and can often be related to the smoothness of the model’s input parameters. For the elliptic problem [8], it was shown in [14] (Lemma 3.2) that if

$$||\partial^l_{\vec{y}} u(y)||_{L^p} \leq \theta_l, \quad ||\partial^l_{\vec{y}} f(y)||_{L^2} \leq \theta_l, \quad \text{a.e. on } \Gamma,$$

where $0 < \theta_l < \infty$ is independent of $\vec{y} = (y_n^1, y_n^2) \in \Gamma$, then $u_h \in C_{\text{mix}}^k(\Gamma, H^1(D))$. The above condition is readily satisfied by standard finite noise approximations of the coefficients. In [15] (and later in [16]) it was shown that for functions in $C_{\text{mix}}^k$, the interpolation error for the isotropic Smolyak approximation based on global Lagrange polynomials has upper bound of the form

$$||u - I_M u||_{C^0(\Gamma, W)} \leq cM^{-k} \log(M)^{(k+2)(N-1)+1}||u||_{\text{mix},k}. \quad (17)$$

The works [10, 18] make use of piecewise linear nodal basis functions with local support to interpolate functions with limited smoothness, obtaining an estimate on the sampling error for functions in $C_{\text{mix}}^2(\Gamma, W(D))$ of the form,

$$||u - I_M u||_{C^0(\Gamma, W)} \leq cM^{-2} \log(M)^{(N-1)} ||u||_{\text{mix},2}. \quad (18)$$

The hierarchical construction of the piecewise linear sparse grid interpolant also lends itself well to adaptive refinement through the use the hierarchical surplus as an indicator of discontinuity. This approach has been extended to constructions using wavelets (see [23]).

The convergence rate in (17) was improved in [16] to an algebraic rate for integrands within a special class of functions $C_{\text{mix}}^\infty(\Gamma, W(D))$ that have analytic extension in each direction. In particular, $u \in C^0(\Gamma, W(D))$ is a member of $C_{\text{mix}}^\infty(\Gamma, W(D))$ if for every $y = (y_n^1, y_n^2) \in \Gamma$, $n = 0, 1, \ldots, N$. For the purposes of error estimation for sparse grid methods, the integrand $u_h$ is often required to have bounded mixed derivatives of order $k \in \mathbb{N}_0$, i.e. to belong to the space

$$C_{\text{mix}}^k(\Gamma, W(D)) = \left\{ w : \Gamma \rightarrow W(D) : ||w||_{\text{mix},k} := \max_{\gamma \in \Gamma, r \leq k} ||D^r w(y)||_W < \infty \right\},$$

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$$||\partial^l_{\vec{y}} u(y)||_{L^p} \leq \theta_l, \quad ||\partial^l_{\vec{y}} f(y)||_{L^2} \leq \theta_l, \quad \text{a.e. on } \Gamma,$$

where $0 < \theta_l < \infty$ is independent of $\vec{y} = (y_n^1, y_n^2) \in \Gamma$, then $u_h \in C_{\text{mix}}^k(\Gamma, H^1(D))$. The above condition is readily satisfied by standard finite noise approximations of the coefficients. In [15] (and later in [16]) it was shown that for functions in $C_{\text{mix}}^k$, the interpolation error for the isotropic Smolyak approximation based on global Lagrange polynomials has upper bound of the form

$$||u - I_M u||_{C^0(\Gamma, W)} \leq cM^{-k} \log(M)^{(k+2)(N-1)+1}||u||_{\text{mix},k}. \quad (17)$$

The works [10, 18] make use of piecewise linear nodal basis functions with local support to interpolate functions with limited smoothness, obtaining an estimate on the sampling error for functions in $C_{\text{mix}}^2(\Gamma, W(D))$ of the form,

$$||u - I_M u||_{C^0(\Gamma, W)} \leq cM^{-2} \log(M)^{(N-1)} ||u||_{\text{mix},2}. \quad (18)$$

The hierarchical construction of the piecewise linear sparse grid interpolant also lends itself well to adaptive refinement through the use the hierarchical surplus as an indicator of discontinuity. This approach has been extended to constructions using wavelets (see [23]).

The convergence rate in (17) was improved in [16] to an algebraic rate for integrands within a special class of functions $C_{\text{mix}}^\infty(\Gamma, W(D))$ that have analytic extension in each direction. In particular, $u \in C^0(\Gamma, W(D))$ is a member of $C_{\text{mix}}^\infty(\Gamma, W(D))$ if for every $y = (y_n^1, y_n^2) \in \Gamma$, $n =
admits an analytic extension in [16] then uses these estimates to bound the Smolyak interpolation by

\[ |u_\text{mix, oo}| := \max_{z \in \mathbb{C} : \text{dist}(z, \Gamma_n) \leq \tau_n} |u(z)| c_0(\Gamma_n^*, W(D)) \]

so that

\[ \|u\|_{\text{mix, oo}} := \max_{n=1, \ldots, N} |u_\text{mix, oo}|. \]

For the elliptic equation (8), the following mild assumption on coefficients guarantees that \( u \in C_\text{mix}(\Gamma, H^1(D)) \) (see [14], Lemma 3.2).

**Assumption 2.** Assume that for every \( y = (y_n, y_n^*) \in \Gamma \), there is a constant \( \theta_n < \infty \) so that

\[ \frac{\|\partial_\gamma a(y)\|}{\|a(y)\|} \leq \theta_n^k k! \quad \text{and} \quad \frac{\|\partial_\gamma f(y)\|}{1 + \|f(y)\|} \leq \theta_n^k k!, \]

for all \( k \in \mathbb{N}^+ \).

Although the sampling error estimates derived in [16] depend on the norms \( |u|_{\text{mix, oo}} \), where \( n = 1, \ldots, N \), these were subsumed into a scaling constant. For our purposes, however, it is necessary for them to appear explicitly in the error estimate. The following lemma therefore indicates how the derivations in [16] can be modified to achieve this.

**Lemma 1.** Let \( \psi(N)u \) be the Smolyak interpolant of the function \( u \) contained in \( C_\text{mix}(\Gamma, W(D)) \), based on Clenshaw-Curtis abscissas and Lagrange polynomials. The interpolation error then satisfies

\[ \|u - \psi(N)u\|_{C_0(\Gamma, W)} \leq c M^{-\mu_2} \max\{\|u\|_{\text{mix, oo}}, \|u\|_{\text{mix, oo}}^N\}, \]

for constants \( c \geq 1 \) and \( \mu_2 > 0 \).

**Proof.** The estimation of the interpolation error of \( u \) over the domain \( \Gamma \subset \mathbb{R}^N \) is based on its one-dimensional counterparts. Indeed it was shown in [10] (see also [14], Lemma 4.4) that for functions \( u \in C_\text{mix}(\Gamma, W(D)) \),

\[ \|u - \psi(N)u\|_{C_0(\Gamma, W)} \leq C_{\text{lin}} e^{-\sigma^2 N}, \]

where \( \sigma = \max_{n=1, \ldots, N} \frac{1}{2} \log \left( \frac{2r_n}{|I_n|} + 1 + \frac{4r_n^2}{|I_n|^2} \right) \) and \( C = \frac{4 \epsilon_1 + 1}{\pi \sigma_{\epsilon_1} \sigma_{\epsilon_2}} \|u\|_{\text{mix, oo}} \). Lemma 3.3 in [16] then uses these estimates to bound the Smolyak interpolation by

\[ \|u - \psi(N)u\|_{C_0(\Gamma, W)} \leq \frac{1}{2} \sum_{n=1}^{N} (2C)^n \sum_{\left[ i \right]_{\epsilon_1}^{\epsilon_2} = 1} \left( \prod_{i=1}^{n} i_{\epsilon_1} \right) e^{-\sigma^2 N} 2^{-n}, \]

\[ \leq \max\{\|u\|_{\text{mix, oo}}, \|u\|_{\text{mix, oo}}^N\} \frac{1}{2} \sum_{n=1}^{N} (2C)^n \sum_{\left[ i \right]_{\epsilon_1}^{\epsilon_2} = 1} \left( \prod_{i=1}^{n} i_{\epsilon_1} \right) e^{-\sigma^2 N} 2^{-n}. \]
The remainder of the derivation in [16] (Lemma 3.4, and Theorems 3.6 and 3.9) remains unchanged, except for the replacement of the constant $C$ in with $\widetilde{C}$ and the addition of the term $\max\{\|u\|_{\text{mix},\infty},\|u\|^{N}_{\text{mix},\infty}\}$. Theorem 3.9 in [16] then asserts

$$\|u - I_M u\|_{C^0(\Gamma; W(D))} \leq cM^{-\mu_2\gamma} \max\{1, C_1(\sigma, \delta^*)\}^N,$$

where

$$c = \frac{C_1(\sigma, \delta^*)e^{\sigma}}{|1 - C_1(\sigma, \delta^*)|} \max\{1, C_1(\sigma, \delta^*)\}^N,$$

$$\mu_2 = \frac{\sigma}{1 + \log(N)},$$

and $C_1(\sigma, \delta^*)$ is defined in [16], Equation (3.12). \hfill \Box

In summary, the sampling error estimates (17), (18) and (20) discussed in this section can therefore all be written in the form

$$\|u - I_M u\|_{W} \leq c_3 \log(M) \mu_1 - \mu_2 \varphi(u_h),$$

where $c_3 \geq 1$, $\mu_1 \geq 0$, and $\mu_2 > 0$ and $\varphi : W(D) \to [0, \infty)$ satisfies $\varphi(u_h) \to 0$ for any sequence $u_n \to 0$ in $C^{(m)}_{\text{mix}}(\Gamma; W(D))$ for $k \in \mathbb{N} \cup \{\infty\}$.

3. The Efficiency of Sampling Methods

A useful indicator of an algorithm’s efficiency is its $\varepsilon$-cost $C_\varepsilon$, defined as the amount of computational effort required to reach a given level of accuracy $\varepsilon > 0$. This effort can be measured in terms of the number of floating point operations or CPU time and is estimated based on a priori error estimates. We now proceed to estimate the $\varepsilon$-cost of the sampling schemes discussed above. In general, the total cost $C(Q_{M,h})$ of computing the estimate $Q_{M,h}$ is approximately

$$C(Q_{M,h}) = \sum_{m=1}^{M} C^{(m)}_h,$$

where $C^{(m)}_h$ is the cost of computing the $m^{th}$ sample at spatial refinement level $h$. If the cost of a system solve is the same for all sample paths, i.e. $C^{(m)}_h = C_h$ for $m = 1, \ldots, M$ then this sum simplifies to

$$C(Q_{M,h}) = MC_h.$$  \hfill (23)

Sampling methods are fully parallelizable and the cost savings of a parallel implementation can be readily incorporated into this cost estimate. Indeed, if the stochastic simulation is distributed among $N_{\text{batch}}$ processors then the total cost is simply scaled by $\frac{1}{N_{\text{batch}}}$. In addition, we assume here that $C_h$ grows polynomially with decreasing spatial refinement level $h$, i.e. there are constants $h_0 > 0$, $c_2 \geq 1$ and $\gamma > 0$, so that

$$c_2 h^{-\gamma} \leq C_h \quad \text{for all } 0 < h < h_0.$$  \hfill (A2)

The $\varepsilon$-cost for a sampling method can then be bounded by determining the lowest values of $h$ and $M$ for which both the spatial error and the sampling error are less than $\varepsilon$, and substituting these values into (23), using (A2). Indeed, supposing the spatial discretization error has upper bound of
the form \( \|u - u_h\|_{L^2(\Gamma,w)} \leq c_1 h^\alpha \) for some \( c_1 \geq 1, \alpha > 0 \), then \( h < \frac{1}{c_1} \varepsilon^{\frac{1}{\alpha}} \) ensures that the spatial refinement error is within the tolerance level \( \frac{\varepsilon}{c_1} \), and hence

\[
C_h \geq c_2 (2c_1)^\gamma \varepsilon^{-\frac{\varepsilon}{c_1}}.
\]

If the upper bound in the generic sparse grid sampling error (22) doesn’t contain a logarithmic term, i.e. if \( \mu_1 = 0 \), then it readily follows that a sample size \( M \geq (2c_1\varphi(u_h))^\frac{\mu_1}{\gamma} E^{-\frac{\mu_1}{\gamma}} \) guarantees a sampling error within the tolerance level \( \frac{\varepsilon}{c_1} \). In this case, the \( \varepsilon \)-cost is at least

\[
C_{\varepsilon}(Q_M) \geq M C_h \geq (2c_1\varphi(u_h))^\frac{\mu_1}{\gamma} (2c_1)^\gamma E^{-\frac{\mu_1}{\gamma}} = O(\varepsilon^{-\frac{\mu_1}{\gamma}}).
\]

We assume here implicitly that the term \( \varphi(u_h) \) remains more or less unchanged as \( h \to 0^* \), a reasonable assumption if \( u_h \to u \). For the general case when \( \mu_1 > 0 \), the minimal sample size required \( M \) is slightly more involved. We derive such values in the following lemma. Note that for any \( x \in \mathbb{R} \), \( \lceil x \rceil \) denotes the unique integer \( n \), so that \( x \leq n < x + 1 \).

**Lemma 2.** Let \( 0 < \mu_2, \tilde{\mu}_2 \) and \( 0 < \mu_1 \leq \tilde{\mu}_1 \) be constants and suppose \( 0 < \varepsilon < 1 \). If

\[
M = \left\lceil \varepsilon^{-\frac{\mu_1}{\gamma}} \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \right) \right\rceil,
\]

then

\[
M^{\mu_1} \log(M)^{\mu_1} \leq \left( 1 + \frac{\tilde{\mu}_1}{\mu_2} + \frac{1}{\mu_2} \right)^{\mu_1} \varepsilon^{\frac{\mu_1}{\gamma}}.
\]

**Proof.** The definition of the \( \lceil \cdot \rceil \) operation implies

\[
\varepsilon^{-\frac{\mu_1}{\gamma}} \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \right)^{\frac{\tilde{\mu}_1}{\mu_1}} \leq M < \varepsilon^{-\frac{\mu_1}{\gamma}} \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \right)^{\frac{\tilde{\mu}_1}{\mu_1}} + 1
\]

and hence

\[
M^{\mu_1} \leq \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \right)^{\frac{\tilde{\mu}_1}{\mu_1}} \right)^{\mu_1} = \varepsilon^{\frac{\tilde{\mu}_1}{\mu_1}} \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \right)^{\frac{\tilde{\mu}_1}{\mu_1}}.
\]

Moreover, using the inequality \( \log(x) < \frac{x}{s} \) for all \( x, s > 0 \) and the fact that \( \varepsilon < 1 \), we get

\[
\log(M)^{\mu_1} < \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \right)^{\frac{\tilde{\mu}_1}{\mu_1}} + 1 \right)^{\mu_1} \leq \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \right) + 1 \right)^{\mu_1}
\]

\[
< \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \log \left( \varepsilon^{-\frac{\mu_1}{\gamma}} \right) + (e - 1) \varepsilon^{-\frac{\mu_1}{\gamma}} \right)^{\mu_1}
\]

\[
= \left( 1 + \frac{1}{\mu_2} + \frac{\tilde{\mu}_1}{\mu_2} \log(\varepsilon)^{-1} \right)^{\mu_1}.
\]
Combining inequalities (27) and (28) yields
\[
M^{-\mu_2} \log(M)^{\mu_1} \leq \log\left(\varepsilon^{-1}\right)^{\bar{\mu}_1} \left(1 + \frac{1}{\bar{\mu}_2 + \frac{\bar{\mu}_1}{\mu_2}} \log\left(\varepsilon^{-1}\right)\right)^{\bar{\mu}_2} e^{\frac{\bar{\mu}_2}{\mu_2}} \\
= \log\left(\varepsilon^{-1}\right)^{\bar{\mu}_1} \left(\frac{1}{\log(\varepsilon^{-1})} + \frac{1}{\bar{\mu}_2 + \frac{\bar{\mu}_1}{\mu_2}}\right)^{\mu_1} e^{\frac{\bar{\mu}_2}{\mu_2}} \\
\leq \left(1 + \left(\frac{1}{\bar{\mu}_2 + \frac{\bar{\mu}_1}{\mu_2}}\right)^{\mu_1} e^{\frac{\bar{\mu}_2}{\mu_2}}\right). 
\]

**Remark 1.** By replacing \(\varepsilon\) in formula (23) with
\[
\tilde{\varepsilon} := \left(1 + \left(\frac{1}{\bar{\mu}_2 + \frac{\bar{\mu}_1}{\mu_2}}\right)^{\mu_1} e^{\frac{\bar{\mu}_2}{\mu_2}}\right) \varepsilon \leq \varepsilon < 1, \tag{29}\]
we can in fact achieve the upper bound
\[
M^{-\mu_2} \log(M)^{\mu_1} \leq \varepsilon. 
\]

The sample size \(M\) necessary to compute the \(\varepsilon\)-cost when \(\mu_1 > 0\) is therefore of the order
\[
M = O\left(e^{\frac{\mu_1}{\mu_2}} \log(e^{-1})^{\frac{\bar{\mu}_2}{\mu_2}}\right), 
\]
leading to the \(\varepsilon\)-cost
\[
C_\varepsilon(Q_{M,h}) = O\left(e^{\frac{\mu_1}{\mu_2}} \log(e^{-1})^{\frac{\bar{\mu}_2}{\mu_2}}\right). \tag{30}\]

4. Multilevel Sampling

4.1. The Multilevel Algorithm

Let \(\{h_\ell\}_{\ell=0}^L\) be a sequence of spatial discretization parameters giving an increasing level of accuracy and let \(h_L\) be chosen to ensure that the spatial error term in (10) satisfies
\[
\|Q - Q_{h_L}\|_W \leq \frac{\varepsilon}{2}. 
\]

Multilevel quadrature methods are based on an expansion of this fine scale approximation \(G(u_{h_{\ell}})\) as the sum of an initial coarse scale approximation and a series of correction terms, i.e.
\[
G(u_{h_{\ell}}) = G(u_{h_0}) + \sum_{\ell=1}^{L} (G(u_{h_\ell}) - G(u_{h_{\ell-1}})). 
\]

Taking expectations on both sides yields
\[
Q_{h_{\ell}} = Q_{h_0} + \sum_{\ell=1}^{L} (Q_{h_{\ell}} - Q_{h_{\ell-1}}). 
\]
We now further estimate \( Q_{h_c} \) by approximating both the coarse approximation and each correction term in the above sum using a different interpolant, i.e.

\[
Q \approx Q_{\text{MLSC}}^{\text{MLSC}} := Q_{M_0, h_0}^{\text{SC}} + \sum_{\ell=1}^{L} (Q_{M_{\ell}, h_{\ell}}^{\text{SC}} - Q_{M_{\ell-1}, h_{\ell-1}}^{\text{SC}}).
\]  

(31)

Since the stochastic interpolation levels, i.e. the sample sizes \( M_{\ell} \) can be chosen separately for each spatial refinement level, using the multilevel estimate gives us the flexibility to coordinate the sample sizes \( M_0, ..., M_L \) in such a way that more samples are drawn at coarse spatial refinement levels while samples at finer spatial refinement levels are sampled more sparingly, hopefully improving the computational efficiency. For the sake of comparison, we refer to the sampling methods discussed in the previous section as single level sampling methods, since only spatial discretizations at the highest refinement level \( h_L \) are sampled.

The total error for the multilevel estimate can now be decomposed as follows

\[
\|Q - Q_{\text{MLSC}}^{\text{MLSC}}\|_W = \|Q - Q_{h_c}\|_W + \|Q_{h_c} - Q_{M_0, h_0}\|_W + \sum_{\ell=1}^{L} \| (Q_{M_{\ell}, h_{\ell}} - Q_{M_{\ell-1}, h_{\ell-1}}) \|_W.
\]  

(32)

Just as in the total approximation error \((10)\) for single level sampling methods, the error in \((32)\) can thus be decomposed into a spatial discretization error, depending only on \( h_L \), and a multilevel sampling error, quantifying the accuracy with which of the correction terms \( G(u_{h_{\ell}}) - G(u_{h_{\ell-1}}) \) are approximated through interpolation.

The basic multilevel sampling method, based on numerical estimates \( e_L^{\text{space}} \) and \( e_{L}^{\text{sample}} \) of the spatial error and the multilevel sampling error respectively, is outlined in Algorithm 1.

**Algorithm 1: Basic multilevel sampling algorithm**

1. **Input**: Tolerance level \( \varepsilon > 0 \), initial discretization level \( h_0 \)
2. **Output**: Maximum refinement level \( L \), multilevel estimate \( Q_{\text{MLSC}}^{\text{MLSC}} \) of \( Q \)
3. Determine initial sample size \( M_0 \);
4. Generate sample \( \{u_{h_0}(\mathbf{x}), \mathbf{y}^{(m)}\}_{m=1}^{M_0} \) and compute \( Q_{\text{MLSC}}^{\text{MLSC}}(M_0, h_0) = Q_{M_0, h_0}^{\text{SC}} \);
5. Set spatial error estimate \( e_0^{\text{space}} = 1 \), maximum refinement level \( L = 0 \);
6. **while** \( e_L^{\text{space}} > \frac{\varepsilon}{2} \) **do**
7. \( L \leftarrow L + 1 \);
8. Refine the model at new discretization level \( h_L \);
9. **while** \( e_L^{\text{space}} + e_{L}^{\text{sample}} < \varepsilon \) **do** while minimizing the total computational cost \( C(Q_{\text{MLSC}}^{\text{MLSC}}(M_{\ell}, h_{\ell})) \);
10. Generate samples \( \{u_{h_\ell}(\mathbf{y}^{(m)})\}_{m=1}^{M_\ell} \) for \( \ell = 0, ..., L \);
11. Update the multilevel estimate \( Q_{\text{MLSC}}^{\text{MLSC}}(M_{\ell}, h_{\ell}) \);
12. Compute \( e_L^{\text{space}} \);
13. **end**
We elaborate on some of the lines in Algorithm 1 and outline some of the outstanding issues addressed in the remainder of this paper. Traditionally (see [5, 11, 13]), the spatial grid refinement step is achieved by scaling the mesh spacing parameter by a fixed percentage, i.e. \( h_{L+1} = s h_L \) for \( L = 1, 2, \ldots \) and \( 0 < s < 1 \). While this construction is convenient to analyze, it is not necessary for the convergence of the algorithm. In fact, the determination of adaptive mesh refinement strategies in this context is a topic of ongoing research.

In some cases the integrand \( G(I_M u_h) \) is a spatially varying function, defined on some spatial mesh \( T_h \). The computation of the sample correction paths \( G(I_M \ell u_{h-1}^\ell(\vec{y}_m)) - G(I_M \ell u_{h-1}^\ell(\vec{y}_m)) \) (line 8) that are used to update the multilevel estimate (see line 9), requires the spatial interpolation of \( v^m_i \) at points on the refined mesh \( T_{h_\ell} \). In [8], this additional cost is mitigated through the use of hierarchical finite elements [24]. For general spatial domains \( D \), such hierarchical approximations are however not always tractable.

One benefit of using nested grids, such as the Clenshaw-Curtis sparse grid, is that the interpolant \( I_{M_{\ell-1}} u_{h_{\ell-1}} \), computed as the ‘fine’ spatial grid interpolant of the previous correction term, can be used to construct the ‘coarse’ spatial grid interpolant \( I_M u_{h_{\ell-1}} \) of the next correction term. In fact if \( M_{\ell-1} > M_\ell \), which is likely to be the case for the optimal sample sizes, no additional sample paths need to be generated. In contrast, Monte Carlo sampling requires sample paths of correction terms to be independent, which prohibits the re-use of sample paths.

Similar to single level methods, the total cost of computing the multilevel estimate (31) is dominated by the construction of the interpolants, i.e.

\[
C(Q^{ML,SC}_{M_l,h_l}) \approx \sum_{\ell=0}^{L} M_\ell C_\ell, \tag{33}
\]

where \( C_\ell \) is the combined cost of computing the sample paths of \( u_{h_{\ell}}(\vec{y}_m^\ell) \) and \( u_{h_{\ell-1}}(\vec{y}_m^\ell) \) for each \( m = 1, \ldots, M_\ell \).

4.2. The Optimal Allocation Sub-Problem

The determination of optimal sample sizes \( \{M_0, \ldots, M_L\} \) in (31) represents the most important step of Algorithm 1 and can be succinctly formulated as a discrete constrained optimization problem in \( L + 1 \) variables. Since the spatial error is independent of the sample size, this term can be ignored. The sample sizes \( M_0, \ldots, M_L \) should then be chosen so as to minimize the total computational effort, while maintaining a sample error that is within. For convenience, we require both the sampling- and spatial errors to be bounded above by \( \varepsilon/2 \). Written as an optimization problem, line 7 amounts to

\[
\min_{M_0, \ldots, M_L} \sum_{\ell=0}^{L} M_\ell C_\ell, \tag{34}
\]

subject to

\[
\|Q_{h_0} - Q_{SC_{M_0,h_0}}\|_W + \sum_{\ell=1}^{L} \left\| (Q_{h_\ell} - Q_{SC_{h_\ell}}) - (Q_{SC_{M_\ell,h_\ell}} - Q_{SC_{M_\ell,h_{\ell-1}}}) \right\|_W \leq \frac{\varepsilon}{2}.
\]
Like the single-level sampling methods, the multi-level Algorithm 1 is amenable to parallel implementation, the effect of which can be incorporated into the total cost by simply dividing throughout by the batch size $N_{\text{batch}}$. Since the inclusion of this factor does not change the optimization problem (34), we leave it out for simplicity.

As a matter of notational convenience, we define

$$\Delta u_\ell := \begin{cases} u_{h_0} & \text{for } \ell = 0 \\ u_{h_\ell} - u_{h_{\ell-1}} & \text{for } \ell = 1, 2, \ldots, L \end{cases}$$

We want to bound the multilevel sampling error in (32) by an expression involving the interpolation error $\|\Delta u_\ell - I_M\Delta u_\ell\|_{C^0(\Gamma; W)}$ for which we have a priori error estimates, such as (17), (18), or (30). For the coarsest refinement level, $\ell = 0$, this can achieved using Jensen’s inequality together with Assumption 1 yielding

$$\|Q_{h_0} - Q_{MC,h_0}\|_W = \|E[G(u_{h_0}) - G(I_{M_0} u_{h_0})]\|_W \leq E \|G(u_{h_0}) - G(I_{M_0} u_{h_0})\|_W$$

$$\leq \|C_\Gamma\|_W \|u_{h_0} - I_{M_0} u_{h_0}\|_{C^0(\Gamma; W)} \leq \tilde{c}_3 \log(M_0)^{\mu_1} M_0^{\mu_2} \varphi(u_{h_0}).$$

for the appropriate constant $\tilde{c}_3$. To ensure that similar upper bounds hold for the higher order correction terms, we make the following assumption.

**Assumption 3.** Assume that the mapping $G : W(D) \to \tilde{W}(D)$ is continuously Fréchet differentiable.

Note that we try to remain agnostic regarding the smoothness of $G(u_h)$ with respect to the vector $\vec{y} \in \Gamma$, allowing the estimation of the integral $\int G(I_M u_h) \rho(\vec{y}) \, d\vec{y}$ to be treated separately from the interpolation $I_M u_h$ of $u_h$. Recall that $Q_{MC} := \int G(I_M u_h) \rho(\vec{y}) \, d\vec{y}$.

**Lemma 3.** Suppose $u \in C^0(\Gamma, W)$ satisfies (9). Assumption 3 holds, and $Q$ is estimated by the multilevel estimate (33). Then there exist constants $C_{G'} , C_{G''} > 0$ such that for $\ell = 1, 2, \ldots, L$

$$\|Q_{h_\ell} - Q_{h_{\ell-1}}| - (Q_{MC,h_\ell} - Q_{MC,h_{\ell-1}})\|_W \leq (C_{G'} + C_{G''} \|\Delta u_\ell\|_{C^0(\Gamma; W)}) \|\Delta u_\ell - I_M \Delta u_\ell\|_{C^0(\Gamma; W)}$$

$$+ C_{G''} \|\Delta u_\ell\|_{C^0(\Gamma; W)} \|u_{h_{\ell-1}} - I_M u_{h_{\ell-1}}\|_{C^0(\Gamma; W)}$$

**(35)**

**Proof.** For spatial refinement levels $\ell \geq 1$, we use Jensen’s inequality to obtain

$$\|E[G(u_{h_\ell}) - G(u_{h_{\ell-1}}) - E[G(I_M u_{h_\ell}) - G(I_M u_{h_{\ell-1}})]\|_W$$

$$\leq E \|G(u_{h_\ell}) - G(u_{h_{\ell-1}}) - G(I_M u_{h_\ell}) - G(I_M u_{h_{\ell-1}})\|_W$$

$$\leq \|G(u_{h_\ell}) - G(u_{h_{\ell-1}}) - G(I_M u_{h_\ell}) - G(I_M u_{h_{\ell-1}})\|_{C^0(\Gamma; W)}.$$
spaces and the linearity of $I_M$ to obtain

$$G(u_0) - G(u_{h_{-1}}) - (G(I_M u_0) - G(I_M u_{h_{-1}}))$$

$$= \int_0^1 G'(u_{t_{-1}} + t \Delta u_t) \Delta u_t dt - \int_0^1 G'(I_M u_{h_{-1}} + t I_M \Delta u_t) I_M \Delta u_t dt$$

$$= \left( \int_0^1 G'(u_{t_{-1}} + t \Delta u_t) - G'(I_M u_{h_{-1}} + t \Delta u_t) \right) \Delta u_t$$

$$- \left( \int_0^1 G'(I_M u_{h_{-1}} + t I_M \Delta u_t) \right) (\Delta u_t - I_M \Delta u_t)$$

The first term can be further simplified through

$$\left\| \int_0^1 G'(u_{t_{-1}} + t \Delta u_t) - G'(I_M u_{h_{-1}} + t \Delta u_t) dt \right\|_W$$

$$\leq \sup_{t, \tau \in [0,1]} \left\| G''(\tilde{\xi}(s, t)) \right\| \left\| \|u_{h_{-1}} - I_M u_{h_{-1}}\|_W + \|\Delta u_t - I_M \Delta u_t\|_W \right\| \|\Delta u_t\|_W$$

where

$$\tilde{\xi}(t, s) = I_M (u_{h_{-1}} + t \Delta u_t) + s (u_{h_{-1}} - I_M u_{h_{-1}} + t (\Delta u_t - I_M \Delta u_t)).$$

Therefore,

$$\left\| G(u_0) - G(u_{h_{-1}}) - G(I_M u_0) + G(I_M u_{h_{-1}}) \right\|_W$$

$$\leq \sup_{t, \tau \in [0,1]} \left\| G'(I_M u_{h_{-1}} + t I_M \Delta u_t) \right\| \|\Delta u_t - I_M \Delta u_t\|_W$$

$$+ \sup_{t, \tau \in [0,1]} \left\| G''(\tilde{\xi}(s, t)) \right\| \left\| \|u_{h_{-1}} - I_M u_{h_{-1}}\|_W + \|\Delta u_t - I_M \Delta u_t\|_W \right\| \|\Delta u_t\|_W$$

Taking maxima on both sides then produces the bound (35) with

$$C_G = \sup_{t, \tau \in [0,1]} \left\| G'(I_M u_{h_{-1}} + t I_M \Delta u_t) \right\|$$

and

$$C_{G'} = \sup_{t, \tau \in [0,1]} \left\| G''(\tilde{\xi}(s, t)) \right\|.$$

Since $\|\Delta u_t\|_{C[\Gamma, W]} \leq \|\Delta u_t\|_{\text{mix}, k} \leq \varphi(\Delta u_t)$ for $k \in \mathbb{N} \cup \{\infty\}$, we can further bound the error in (35) in terms of the generic sampling error (22). Indeed,

$$(C_G + C_{G'} \|\Delta u_t\|_{C[\Gamma, W]} \|\Delta u_t - I_M \Delta u_t\|_{C[\Gamma, W]} \leq c \log(M_t)^{\nu} M_t^{\mu} \varphi(\Delta u_t)$$

while

$$C_G \|\Delta u_t\|_{C[\Gamma, W]} \|u_{h_{-1}} - I_M u_{h_{-1}}\|_{C[\Gamma, W]} \leq C_G \hat{c}_3 \log(M_t)^{\nu} M_t^{\mu} \varphi(u_0) \varphi(\Delta u_t).$$
Combining these two estimates finally allows us to write

\[ \left\| (Q_{h} - Q_{h,\ell}) - (Q_{M_{\ell},h}^{SC} - Q_{M_{\ell},h,\ell}^{SC}) \right\| \leq c_{3} \log(M_{\ell}^{p_{t}})M_{\ell}^{p_{t}}\varphi(\Delta u_{\ell}). \]  

(36)

The optimal allocation sub-problem (34) can therefore be approximated by

\[ \min_{M_{0}, \ldots, M_{L}} \sum_{\ell=0}^{L} M_{\ell}C_{\ell}, \text{ subject to } c_{3} \sum_{\ell=0}^{L} \log(M_{\ell}^{p_{t}})M_{\ell}^{p_{t}}\varphi(\Delta u_{\ell}) \leq \varepsilon. \]  

(37)

Like the single-level sampling methods, the multi-level Algorithm 1 is amenable to parallel implementation, the effect of which can be incorporated into the total cost by simply dividing throughout by the batch size \( N_{\text{batch}} \). Since the inclusion of this factor does not change the optimization problem (34), we leave it out for simplicity.

In general, problem (34) is not solved exactly, but rather formulae for \( M_{0}, \ldots, M_{L} \) are derived heuristically, either based on the equilibration of errors \([25, 9]\) or on a continuum approximation \([13, 11, 12]\). We pursue the latter approach, i.e. to determine the optimal sample sizes, we assume for the moment that the variables \( M_{0}, \ldots, M_{L} \) are continuous. The continuous optimization problem has relatively few variables, since \( L \) is usually not too large. If in addition, the error estimates are approximated numerically, based on the general form of the generic estimate (22), explicit formulae can be derived for the minimizers \( M_{0}, \ldots, M_{L} \) in problem (7), which are rounded up to the nearest admissible sample sizes. We discuss this ‘binning’ procedure after the optimal sample sizes are derived.

We are now in a position to estimate the optimal sample sizes \( M_{0}, M_{1}, \ldots, M_{L} \) needed for our multilevel algorithm. Again, we find it convenient to differentiate between sampling errors with- and without a logarithmic term.

### 4.3. Optimal Sample Sizes when \( \mu_{1} = 0 \)

If the sampling error estimate in (36) is of the form

\[ \left\| (Q_{h} - Q_{h,\ell}) - (Q_{M_{\ell},h}^{SC} - Q_{M_{\ell},h,\ell}^{SC}) \right\| \leq c_{3} M_{\ell}^{p_{t}}\varphi(\Delta u_{\ell}) \]  

(38)

then optimization problem (37) is given by

\[ \min_{M_{0}, \ldots, M_{L}} \sum_{\ell=0}^{L} M_{\ell}C_{\ell}, \text{ subject to } c_{3} \sum_{\ell=0}^{L} M_{\ell}^{p_{t}}\varphi(\Delta u_{\ell}) \leq \varepsilon. \]  

(39)

Since the cost functional is simply a hyperplane and the constraint set is convex in \( \mathbb{R}^{L+1} \), a unique minimizer of (39) exists and can be readily determined via Lagrange multipliers. Moreover, at the optimum the constraint is clearly active. The Lagrangian then takes form

\[ \mathcal{L}(M_{0}, \ldots, M_{L}; \lambda) := \sum_{\ell=0}^{L} C_{\ell}M_{\ell} + \lambda \left( c_{3} \sum_{\ell=0}^{L} M_{\ell}^{p_{t}}\varphi(\Delta u_{\ell}) - \varepsilon \right), \]
and its stationary points, obtained by letting \( \frac{\partial L}{\partial M_\ell} = 0 \) for \( \ell = 0, \ldots, L \), satisfy

\[
C_\ell = \lambda c_3 \mu_2 M_\ell^{-\mu_1+1} \varphi(\Delta u_\ell) = 0 \Rightarrow M_\ell = \left( \frac{c_3 \lambda \mu_2 \varphi(\Delta u_\ell)}{C_\ell} \right)^{\frac{1}{\mu_1}}.
\]

Enforcing the equality constraint,

\[
\frac{E}{2} = c_3 \sum_{\ell=0}^{L} M_\ell^{-\mu_3} \varphi(\Delta u_\ell) = c_3 \sum_{\ell=0}^{L} \varphi(\Delta u_\ell) \left( \frac{c_3 \lambda \mu_2 \varphi(\Delta u_\ell)}{C_\ell} \right)^{\frac{1}{\mu_1}}
\]

gives

\[
(\lambda \mu_2)^{\frac{1}{\mu_1}} = \left( \frac{2}{E} \sum_{\ell=0}^{L} (c_3 C_\ell \varphi(\Delta u_\ell))^{\frac{1}{\mu_1}} \right)^{\frac{1}{\mu_1}}
\]

and hence

\[
M_\ell = (2c_3 E^{-1})^{\frac{1}{\mu_1}} \left( \sum_{\ell=0}^{L} (C_\ell \varphi(\Delta u_\ell))^{\frac{1}{\mu_1}} \right)^{\frac{1}{\mu_1}} \left( \frac{\varphi(\Delta u_\ell)}{C_\ell} \right)^{\frac{1}{\mu_1}}, \quad \text{for } \ell = 0, \ldots, L. \tag{40}
\]

With this choice of \( M_0, \ldots, M_L \), the total cost satisfies

\[
\sum_{\ell=0}^{L} C_\ell M_\ell = \sum_{\ell=0}^{L} C_\ell (2c_3 E^{-1})^{\frac{1}{\mu_1}} \left( \sum_{\ell=0}^{L} (C_\ell \varphi(\Delta u_\ell))^{\frac{1}{\mu_1}} \right)^{\frac{1}{\mu_1}} \left( \frac{\varphi(\Delta u_\ell)}{C_\ell} \right)^{\frac{1}{\mu_1}}
\]

\[
= (2c_3 E^{-1})^{\frac{1}{\mu_1}} \left( \sum_{\ell=0}^{L} (C_\ell \varphi(\Delta u_\ell))^{\frac{1}{\mu_1}} \right)^{\frac{\mu_1+1}{\mu_1}}. \tag{41}
\]

4.4. **Optimal Sample Sizes when \( \mu_1 > 0 \)**

To obtain the candidate sample sizes \( M_0, \ldots, M_L \), in this case, we write down the optimization problem again, this time with the sampling error involving a logarithmic term

\[
\min_{M_0, \ldots, M_L > 1} \sum_{\ell=0}^{L} C_\ell M_\ell, \quad \text{subject to} \quad c_3 \sum_{\ell=0}^{L} \log(M_\ell)^{\mu_1} M_\ell^{-\mu_3} \varphi(\Delta u_\ell) \leq \frac{E}{2}. \tag{42}
\]

Here we assume that \( \frac{E}{2} \leq \varphi(\delta_0) \). We form the Lagrangian

\[
L(M_0, \ldots, M_L; \lambda) := \sum_{\ell=0}^{L} C_\ell M_\ell + \lambda \left( c_3 \sum_{\ell=0}^{L} \log(M_\ell)^{\mu_1} M_\ell^{-\mu_3} \varphi(\Delta u_\ell) - \frac{E}{2} \right),
\]

whose stationary points satisfy

\[
C_\ell + c_3 \lambda \varphi(\Delta u_\ell) \left( -\mu_2 M_\ell^{-\mu_1+1} \log(M_\ell)^{\mu_1} + \mu_1 \log(M_\ell)^{\mu_1-1} M_\ell^{-\mu_1+1} \right) = 0
\]
and hence
\[
\left( \mu_2 - \frac{\mu_1}{\log(M_1)} \right) M_{\ell}^{(\mu_2+1)} \log(M_\ell)^{\mu_1} = \frac{C_\ell}{A_3 \varphi(\Delta u_\ell)}.
\]
(43)

In order to obtain an idea of what \( \lambda \) should be, we ignore the one term consider the approximation
\[
M_{\ell}^{(\mu_2+1)} \log(M_\ell)^{\mu_1} \approx \frac{C_\ell}{c_3 \varphi(\Delta u_\ell)}.
\]
(44)

We now choose \( \lambda > 0 \) to ensure
\[
L \sum_{\ell=0}^{L} c_3 \varphi(\Delta u_\ell) \left( \frac{C_\ell}{A_3 \varphi(\Delta u_\ell)} \right)^{\frac{\mu_1}{\mu_2+1}} \leq \frac{\varepsilon}{2},
\]
(45)
i.e.
\[
\lambda = \left( \frac{2}{\varepsilon} L \sum_{\ell=0}^{L} c_3 \varphi(\Delta u_\ell) \right)^{\frac{\mu_2+1}{\mu_1}}.
\]
(46)

Note that
\[
\frac{C_\ell}{A_3 \varphi(\Delta u_\ell)} < 1.
\]
If this were not the case, then (45) would imply
\[
\frac{\varepsilon}{2} = \sum_{\ell=0}^{L} c_3 \varphi(\Delta u_\ell) \left( \frac{C_\ell}{A_3 \varphi(\Delta u_\ell)} \right)^{\frac{\mu_1}{\mu_2+1}} \geq \sum_{\ell=0}^{L} \varphi(\Delta u_\ell)
\]
(recall that we have assumed \( c_3 \geq 1 \) w.l.o.g.) and hence \( \varphi(\Delta u_\ell) < \frac{\varepsilon}{2} \) for all \( \ell = 0, \ldots, L \). In particular, \( \varphi(u_0) \leq \frac{\varepsilon}{2} \), which is impossible by assumption. Inspired by Lemma 2, we now choose the sample sizes \( \{ M_\ell \}_{\ell=0}^{L} \) to be
\[
M_\ell = \left( \frac{K_1 C_\ell}{A_3 \varphi(\Delta u_\ell)} \right)^{\frac{\mu_1}{\mu_2+1}} \log \left( \frac{K_1 C_\ell}{A_3 \varphi(\Delta u_\ell)} \right)^{-\frac{\mu_1}{\mu_2+1}},
\]
(47)
where \( K_1 \) is the scaling factor given in (29) and apply Lemma 2 to conclude
\[
M_{\ell}^{\mu_2} \log(M_\ell)^{\mu_1} \leq \left( \frac{C_\ell}{A_3 \varphi(\Delta u_\ell)} \right)^{\frac{\mu_1}{\mu_2+1}}.
\]
(48)

The total multilevel sampling error can now be bounded by
\[
c_3 \sum_{\ell=0}^{L} M_{\ell}^{\mu_2} \log(M_\ell)^{\mu_1} \varphi(\Delta u_\ell) \leq c_3 \sum_{\ell=0}^{L} \varphi(\Delta u_\ell) \left( \frac{C_\ell}{A_3 \varphi(\Delta u_\ell)} \right)^{\frac{\mu_1}{\mu_2+1}} \leq \frac{\varepsilon}{2}.
\]
(49)

19
according to (45). Substituting the expressions for \([M_\ell]_{\ell=0}^L\) into the total cost then gives

\[
\sum_{\ell=0}^L M_\ell C_\ell \leq \sum_{\ell=0}^L C_\ell \left( \frac{K_\ell C_\ell}{\lambda C_3 \varphi(\Delta u_\ell)} \right)^{\frac{1}{2+\gamma}} \log \left( \frac{K_\ell C_\ell}{\lambda C_3 \varphi(\Delta u_\ell)} \right)^{\frac{1}{2+\gamma}} + 1 \\
eq \left( \frac{c_3}{K_1} \right)^{\frac{1}{2+\gamma}} \lambda^{\frac{1}{2+\gamma}} \sum_{\ell=0}^L \left( C_\ell^2 \varphi(\Delta u_\ell) \right)^{\frac{1}{2+\gamma}} \log \left( \frac{K_\ell C_\ell}{\lambda C_3 \varphi(\Delta u_\ell)} \right)^{\frac{1}{2+\gamma}} + \sum_{\ell=0}^L C_\ell. \tag{50}
\]

In order to make use of formulae (40) and (47) in Algorithm 1, the sample sizes \(M_0, \ldots, M_L\) must first be rounded up, either to the nearest integer in the case of Monte Carlo sampling, or to the size of the sparse grid on the next refinement level \(\nu\) in the case of sparse grid stochastic collocation. Since the number of additional sample points needed for the latter sampling scheme grows increasingly with increasing \(\nu\), especially in high dimensions \(N\), this ‘binning’ could add needlessly to the cost. Let \(M_{0}^{\text{ext}}, \ldots, M_{L}^{\text{ext}}\) be the sample sizes on the next stochastic refinement level \(\nu\) and \(M_{0}^{\text{rev}}, \ldots, M_{L}^{\text{rev}}\) be those on the previous level \(\nu - 1\). The effect of ‘binning’ can be mitigated by sorting \(|M_\ell|_{\ell=0}^L\) in ascending order according to the cost \((M_\ell - M_{\ell}^{\text{rev}}) C_\ell\) and rounding up the \(M_\ell\)’s with lowest cost incrementally, while rounding down the others until the sampling error estimate is within tolerance.

The derivations for the optimal sample sizes \(M_1, \ldots, M_L\) are based on the approximation of problems (39) and (42) by their continuous counterparts, as well as other, heuristic approximations, such as (44). In order to to show that the multilevel algorithm leads to an improvement in efficiency over related single level methods, we need to determine its \(\varepsilon\)-cost. Theorem 1 accomplishes this. Its proof hinges on the fact that

\[
\varphi(\Delta u_\ell) \leq c_4 h_\ell^\beta
\]

for some \(\beta > 0\) and \(c_4 \geq 1\). Therefore the sampling error for numerical integration of the correction terms \(\Delta u_\ell\), decreases as the spatial refinement level \(\ell\) increases. If the finite element approximation converges in mean square, this condition can easily be shown to hold for Monte Carlo sampling, but it requires a proof for Lagrange interpolation, when \(\varphi(\cdot) = \|\cdot\|_{\text{max},k}\). The following lemma shows that under the stricter regularity Assumption 4 and under piecewise linear finite element approximation, such estimates are also possible in this case.

**Assumption 4.** Assume that \(a(\tilde{y}) \in C^1(D), f(\tilde{y}) \in L^2(D)\) a.e. on \(\Gamma\) and that

\[
\|\hat{\varphi}_{\nu,0} a(\tilde{y})\|_{L^\infty(D)} \leq \frac{a_{\text{min}}}{C_{\text{reg}}} \left( \frac{\theta_0}{8} \right)^k \text{ and } \|\hat{\varphi}_{\nu,0} \nabla a(\tilde{y})\|_{L^\infty(D)} \leq \sqrt{a_{\text{min}}} \left( \frac{\theta_0}{8} \right)^k!
\]

while

\[
\|\hat{\varphi}_{\nu,0} f(\tilde{y})\|_{L^2(D)} \leq \frac{a_{\text{min}}}{C_p} (1 + \|f(\tilde{y})\|_{L^2(D)}) \left( \frac{\theta_0}{4} \right)^k!
\]

where \(a_{\text{min}} \leq \sqrt{a_{\text{min}}} < 1\) w.l.o.g., and \(C_{\text{reg}} \geq 1\) is a constant related to the spatial regularity of \(u\) and \(C_p \geq 1\) is a Poincaré constant.

**Lemma 4.** Suppose the parameters \(a\) and \(f\) appearing in the elliptic equation (9) satisfy Assumption 4 and also that \(ht \leq C_{\text{refine}} h_{\ell-1}\) for \(\ell = 0, \ldots, L\). Then there exists a constant \(c_4 \geq 1\) so
that

\[ \|\Delta u_\ell\|_{\text{mix}, \infty} \leq c_{\ell} h_\ell \quad \text{for} \quad k \in \mathbb{N} \cup \{\infty\}, \quad \ell = 1, 2, \ldots \]

**Proof.** It was shown in [14] (Lemma 4.4) that for every \( \vec{y} = (y_n, \vec{y}_n) \in \Gamma \), the \( k \)th derivatives \( \partial_{y_n}^k u \), \( k \in \mathbb{N}_0 \), are well defined as solutions of the variational problem:

\[
B(\vec{y}, \partial_{y_n}^k u, w) = -\sum_{l=1}^k \partial_{y_n}^l B(\vec{y}, \partial_{y_n}^{l-1} u, w) + \partial_{y_n}^k f(\vec{y}), \quad \forall w \in H_0^1(D), \quad (51)
\]

where

\[
B(\vec{y}, u, w) = \int_D a(\vec{y}) \nabla u \cdot \nabla w \, dx, \quad \text{and} \quad (f(\vec{y}), w) = \int_D f(\vec{y}) w \, dx, \quad \forall u, w \in H_0^1(D).
\]

Moreover, they can be used to define a power series expansion \( u : \mathbb{C} \to C^k(\Gamma_n; H_0^1(D)) \),

\[
u(x, z, \vec{y}_n) = \sum_{k=0}^\infty \frac{(z - y_n)^k}{k!} \partial_{y_n}^k u(x, y_n, \vec{y}_n)
\]

that converges whenever \( z \in \Sigma(\Gamma_n, \tau_n) = \{ z \in \mathbb{C} : |z - y_n| \leq \tau_n < 1/(2\theta_n) \} \). The same construction holds for the Galerkin projection \( u_h \) of \( u \), in which case the derivatives \( \partial_{y_n}^k u_h \) satisfy \( (51) \) on \( W_h(D) \subset H_0^1(D) \). It then follows readily that \( \Delta u_\ell \) has the power series expansion

\[
\Delta u_\ell(x, z, \vec{y}_n) = \sum_{k=0}^\infty \frac{(z - y_n)^k}{k!} \partial_{y_n}^k \Delta u_\ell(x, y_n, \vec{y}_n), \quad \forall |z - y_n| \leq \tau_n
\]

and that to estimate \( \|\Delta u\|_{\text{mix}, \infty} \) requires bounding the terms \( \|\partial_{y_n}^k \Delta u_\ell(y)\|_{H_0^1} \) for \( k \in \mathbb{N}_0 \). Let \( \left( \partial_{y_n}^k u \right)_h \) denote the Galerkin projection of \( \partial_{y_n}^k u \) in \( (51) \), i.e.

\[
B(\vec{y}, \left( \partial_{y_n}^k u \right)_h, w) = -\sum_{l=1}^k \left( \frac{l}{l} \right) \partial_{y_n}^l B(\vec{y}, \partial_{y_n}^{l-1} u, w) + \partial_{y_n}^k f(\vec{y}), \quad \forall w \in W_h(D). \quad (52)
\]

The approximation error \( \|\partial_{y_n}^k u - \partial_{y_n}^k u_h\|_{H_0^1} \) for a generic spatial discretization level \( h > 0 \) can be decomposed into

\[
\|\partial_{y_n}^k (u - u_h)\|_{H_0^1} \leq \|\partial_{y_n}^k u - \left( \partial_{y_n}^k u \right)_h\|_{H_0^1} + \|\left( \partial_{y_n}^k u \right)_h - \partial_{y_n}^k u_h\|_{H_0^1}.
\]

Moreover, equations \( (51) \) and \( (52) \) imply

\[
a_{\min}(\|\partial_{y_n}^k u - \partial_{y_n}^k u_h\|_{H_0^1}^2) = -\sum_{l=1}^k \left( \frac{l}{l} \right) \partial_{y_n}^l B(\vec{y}, \partial_{y_n}^{l-1} (u - u_h), \left( \partial_{y_n}^k u \right)_h - \partial_{y_n}^k u_h)
\]

\[
\leq \sum_{l=1}^k \left( \frac{l}{l} \right) \|\partial_{y_n}^k a(\vec{y})\|_{L^\infty(D)} \|\partial_{y_n}^{l-1} (u - u_h)\|_{H_0^1(D)} \|\left( \partial_{y_n}^k u \right)_h - \partial_{y_n}^k u_h\|_{H_0^1} \quad (53)
\]

21
On the other hand, it follows readily from Céa’s Lemma and the appropriate finite element interpolation theorem (see e.g. [19], Chapter 4) that
\[
\left\| (\partial_{\mathcal{S}_u}^k u)^{D} - \partial_{\mathcal{S}_u}^k u \right\|_{H^1(D)} \leq \frac{1}{\sqrt{\Delta_{\min}} \eta} \min_{w \in W_h(D)} \| \partial_{\mathcal{S}_u}^k u - w \|_{H^1(D)} \leq \frac{C_{\text{mesh}}}{\sqrt{\Delta_{\min}}} h \| \partial_{\mathcal{S}_u}^k u \|_{H^2},
\]
(54)
where the constant \( C_{\text{mesh}} > 0 \) depends only on the triangulation \( T_h \). Combining estimates (53) and (54) then gives the recursively defined error estimate
\[
\| \partial_{\mathcal{S}_u}^k (u - u_h) \|_{H^1(D)} \leq \frac{1}{\Delta_{\min}} \sum_{l=1}^k \left( \sum_{i=1}^l \right) \| \partial_{\mathcal{S}_u}^i a(\tilde{\gamma}) \|_{L^\infty} \| \partial_{\mathcal{S}_u}^{k-i} (u - u_h) \|_{H^1} + \frac{C_{\text{mesh}}}{\Delta_{\min}} h \| \partial_{\mathcal{S}_u}^k u \|_{H^2}.
\]
(55)
We turn first to the norm \( \| \partial_{\mathcal{S}_u}^k u \|_{H^1(D)} \). Since \( a(\tilde{\gamma}) \in C^1(D), f(\tilde{\gamma}) \in L^2(D) \) and \( \partial D \in C^2 \), elliptic regularity theory asserts that \( \| u \|_{H^1(D)} \leq C_{\text{reg}} \| f(\tilde{\gamma}) \|_{L^2(D)} \) for an appropriate constant \( C_{\text{reg}} > 0 \) that is independent of \( u \) and \( f \). To bound the \( H^2 \)-norms of the higher order derivatives \( \partial_{\mathcal{S}_u}^k u \), \( k \in \mathbb{N} \), we proceed inductively. Suppose \( \| \partial_{\mathcal{S}_u}^{k-l} u \|_{H^2} < \infty \) for \( l = 1, \ldots, k \). Then the right hand side of (51) can be rewritten as
\[
- \sum_{l=1}^k \left( \sum_{i=1}^l \right) \partial_{\mathcal{S}_u}^i B(\tilde{\gamma}, \partial_{\mathcal{S}_u}^{k-i} u, w) + (\partial_{\mathcal{S}_u}^k f(\tilde{\gamma}), w)
\]
\[
= \int \left( \sum_{l=1}^k \left( \sum_{i=1}^l \right) \partial_{\mathcal{S}_u}^i \nabla a(\tilde{\gamma}) \cdot \nabla \partial_{\mathcal{S}_u}^{k-i} u + \partial_{\mathcal{S}_u}^i a(\tilde{\gamma}) \Delta \partial_{\mathcal{S}_u}^{k-i} u + \partial_{\mathcal{S}_u}^k f(\tilde{\gamma}) \right) w \ dx,
\]
through integration by parts. Moreover
\[
\left\| \sum_{l=1}^k \left( \sum_{i=1}^l \right) \partial_{\mathcal{S}_u}^i \nabla a(\tilde{\gamma}) \cdot \nabla \partial_{\mathcal{S}_u}^{k-i} u + \partial_{\mathcal{S}_u}^i a(\tilde{\gamma}) \Delta \partial_{\mathcal{S}_u}^{k-i} u + \partial_{\mathcal{S}_u}^k f(\tilde{\gamma}) \right\|_{L^2}
\]
\[
\leq \sum_{l=1}^k \left( \sum_{i=1}^l \right) \left( \| \partial_{\mathcal{S}_u}^i \nabla a(\tilde{\gamma}) \|_{L^\infty} \| \partial_{\mathcal{S}_u}^{k-i} u \|_{H^1} + \| \partial_{\mathcal{S}_u}^i a(\tilde{\gamma}) \|_{L^\infty} \| \partial_{\mathcal{S}_u}^{k-i} u \|_{H^1} + \| \partial_{\mathcal{S}_u}^k f(\tilde{\gamma}) \|_{L^2} \right) + \| \partial_{\mathcal{S}_u}^k f(\tilde{\gamma}) \|_{L^2} < \infty,
\]
and hence by regularity
\[
\| \partial_{\mathcal{S}_u}^k u \|_{H^2} \leq C_{\text{reg}} \sum_{l=1}^k \left( \sum_{i=1}^l \right) \| \partial_{\mathcal{S}_u}^i a(\tilde{\gamma}) \|_{L^\infty} \| \partial_{\mathcal{S}_u}^{k-i} u \|_{H^1} + \| \partial_{\mathcal{S}_u}^k f(\tilde{\gamma}) \|_{L^2},
\]
(56)
\[
C_{\text{reg}} \sum_{l=1}^k \left( \sum_{i=1}^l \right) \| \partial_{\mathcal{S}_u}^i \nabla a(\tilde{\gamma}) \|_{L^\infty} \| \partial_{\mathcal{S}_u}^{k-i} u \|_{H^1} + \| \partial_{\mathcal{S}_u}^i a(\tilde{\gamma}) \|_{L^\infty} \| \partial_{\mathcal{S}_u}^{k-i} u \|_{H^1} + \| \partial_{\mathcal{S}_u}^k f(\tilde{\gamma}) \|_{L^2},
\]
(57)
where \( \| \partial_{\mathcal{S}_u}^k u \|_{H^2} \) can be shown to satisfy
\[
\| \partial_{\mathcal{S}_u}^k u \|_{H^1(D)} \leq \sum_{l=1}^k \left( \sum_{i=1}^l \right) \frac{\| \partial_{\mathcal{S}_u}^i a(\tilde{\gamma}) \|_{L^\infty} \| \partial_{\mathcal{S}_u}^{k-i} u \|_{H^1}}{\Delta_{\min}} + \frac{C_{P}}{\Delta_{\min}} \| \partial_{\mathcal{S}_u}^k f(\tilde{\gamma}) \|_{L^2},
\]
(58)
by virtue of (51), where \( C_{P} > 0 \) is the appropriate Poincaré constant. Note that both (55) and
as well as \( \text{(58)} \) involve inequalities that are recursively defined. The following fact provides a means by which such inequalities can be resolved and is used repeatedly in sequel. Let \( c, \theta > 0 \) be constants and \( R_k, R_{k-1}, \ldots \) a sequence of numbers. If, for \( k = 1, 2, \ldots, R_k \) satisfies
\[
R_k \leq \sum_{i=1}^{k} \theta R_{k-i} + \theta^k c \quad \text{then} \quad R_k \leq \sum_{i=1}^{k} \theta^i R_{k-i} + \theta^k c \leq \frac{1}{2}(2\theta)^k(R_0 + c).
\] (59)

Since Assumption 4 implies \( \|\partial^{k}_\alpha \alpha(\vec{y})\|_{L^\infty} \leq \sqrt{\alpha_{\min}(\theta/4)^k}k! \)
and \( \|\partial^{k}_\alpha f(\vec{y})\|_{L^\infty} \leq (1 + \|f(\vec{y})\|_{L^\infty}) \min(1, (\frac{\alpha_{\min}}{C_p})(\theta/4)^k)k! \), inequality \( \text{(58)} \) gives rise to
\[
\frac{|\partial^{k}_\alpha u|_{H^k}}{k!} \leq \sum_{i=1}^{k} \left( \frac{\theta}{4} \right)^i \frac{|\partial^{k-i}_\alpha u|_{H^{k-i}}}{(k-i)!} + \left( \frac{\theta}{4} \right)^k (1 + \|f(\vec{y})\|_{L^\infty})
\leq \left( \frac{\theta}{2} \right)^k \frac{1}{2} \left( \|u|_{H^k} + 1 + \|f(\vec{y})\|_{L^\infty} \right)
\]
while \( \|\partial^{k}_\alpha \nabla u(\vec{y})\|_{L^\infty} \leq \frac{1}{c_{\text{reg}}^2} (\theta/4)^k k! \). together with \( \text{(59)} \) imply that expression \( \text{(57)} \) can also be bounded above by
\[
k! \sum_{i=1}^{k} \left( \frac{\theta}{4} \right)^i \frac{|\partial^{k-i}_\alpha u|_{H^{k-i}}}{(k-i)!} + k! \left( \frac{\theta}{4} \right)^k (1 + \|f(\vec{y})\|_{L^\infty}) \leq k! \left( \frac{\theta}{2} \right)^k \frac{1}{2} \left( \|u|_{H^k} + 1 + \|f(\vec{y})\|_{L^\infty} \right).
\] (60)

Substituting \( \text{(60)} \) into \( \text{(57)} \) and noting \( \|\partial^{k}_\alpha \alpha(\vec{y})\|_{L^\infty} \leq \frac{c_{\text{reg}}}{\sqrt{\alpha_{\min}}}(\theta/4)^k k! \) yields
\[
\frac{|\partial^{k}_\alpha u|_{H^k}}{k!} \leq \sum_{i=1}^{k} \left( \frac{\theta}{2} \right)^i \frac{|\partial^{k-i}_\alpha u|_{H^{k-i}}}{(k-i)!} + \left( \frac{\theta}{2} \right)^k \frac{1}{2} \left( \|u|_{H^k} + 1 + \|f(\vec{y})\|_{L^\infty} \right)
\leq \left( \frac{\theta}{2} \right)^k \left( \left( \frac{C_{\text{reg}}}{2} + \frac{C_p}{4\alpha_{\min}} + 1 \right) \|f(\vec{y})\|_{L^\infty} + 1 \right).
\] (61)

Finally, noting that \( \|\partial^{k}_\alpha \alpha(\vec{y})\|_{L^\infty} \leq a_{\min}(\theta/4)^k \), substituting \( \text{(61)} \) into \( \text{(58)} \) and using \( \text{(59)} \) gives
\[
\frac{|\partial^{k}_\alpha (u - u_0)|_{H^k}}{k!} \leq \sum_{i=1}^{k} \left( \frac{\theta}{2} \right)^i \frac{|\partial^{k-i}_\alpha (u - u_0)|_{H^{k-i}}}{(k-i)!} + \theta^k \hbar \tilde{c}_4 \leq h(2\theta)^k \left( \tilde{c}_4 + \frac{C_{\text{mesh}} C_{\text{reg}}}{\sqrt{\alpha_{\min}}} \right),
\]
where \( \tilde{c}_4 = \frac{C_{\text{mesh}}}{\sqrt{\alpha_{\min}}} \left( \left( \frac{C_{\text{mesh}}}{2} + \frac{C_p}{4\alpha_{\min}} + 1 \right) \|f(\vec{y})\|_{L^\infty} + 1 \right) \). Consequently,
\[
\|\partial^{k}_\alpha \Delta u|_{H^k} \leq \|\partial^{k}_\alpha (u_0 - u)||_{H^k} + \|\partial^{k}_\alpha (u_{n-1} - u)||_{H^k} \leq k! c_4 (2\theta)^k \hbar \tilde{c}_4,
\]
where \( c_4 = \frac{1}{2} \left( \tilde{c}_4 + \frac{C_{\text{mesh}} C_{\text{reg}}}{\sqrt{\alpha_{\min}}} \right) \), and hence
\[
\|\Delta u|_{H^k} \leq \max_{n=1, \ldots, N} \max_{h \leq k} \|\partial^{k}_\alpha \Delta u|_{H^k} \leq k! c_4 (2\theta)^k \hbar \tilde{c}_4.
\]
Theorem 1 (Efficiency of Multilevel Sampling Methods). Suppose $h_t := h_0s^{-t}$ and let the tolerance satisfy $0 < \varepsilon < \min(2\varphi(y_0), 1/\varepsilon)$. Suppose further that there are constants $\alpha, \gamma, \mu_2, \beta > 0$, $\mu_1 \geq 0$, and $c_1, c_2, c_3, c_4 > 0$ so that

(A1) $\|Q - Q_{h_t}\|_{\infty} \leq c_1 h^\alpha$,

(A2) $C_h \leq c_2 h^{-\gamma}$,

(A3) $\left\| (Q_{h_t} - Q_{h_{t-1}}) - (Q_{M_t,h_t}^{SC} - Q_{M_t,h_{t-1}}^{SC}) \right\|_{\infty} \leq c_3 \log(M_t)^{\mu_1} M_t^{\mu_2} \varphi(\Delta u_t)$, and

(A4) $\varphi(\Delta u_t) \leq c_4 h_{\ell}^\beta$.

We assume throughout that $\alpha < \gamma \mu_2$ and further, without loss of generality (w.l.o.g.), that $c_1 \geq 1$ for $i = 1, \ldots, 4$. Then there exists an $L \in \mathbb{N}$ and $\{M_t\}_{t=0}^L \subset \mathbb{N}^k$ so that the resulting multilevel estimate $Q_{(M_t),[h_t]}$ approximates $Q$ with a total error of

$$\|Q - Q_{(M_t),[h_t]}\| \leq \varepsilon,$$

while the total computational cost $C(Q_{(M_t),[h_t]})$ satisfies

$$C(Q_{(M_t),[h_t]}) \leq \begin{cases} d_1 \varepsilon^{-\frac{\gamma \mu_2}{\beta}} \log(\varepsilon^{-1})\frac{\varepsilon^2}{\alpha}, & \text{if } \beta < \gamma \mu_2 \\ d_2 \varepsilon^{-\frac{\alpha}{\beta}} \log(\varepsilon^{-1})^{1 + \frac{\mu_2}{\beta}}, & \text{if } \beta = \gamma \mu_2 \\ d_3 \varepsilon^{-\frac{\alpha}{\beta}}, & \text{if } \beta > \gamma \mu_2 \end{cases}$$ (62)

where the constants $d_i$ may differ according to whether $\mu_1 = 0$ or $\mu_1 > 0$.

Proof. We first choose the maximum spatial refinement level $L$ large enough to ensure that the spatial approximation error satisfies

$$\|Q - Q_{h_L}\|_{\infty} \leq \frac{\varepsilon}{2}.$$

Under Assumption (A1), it suffices to take $L$ to be the smallest integer for which

$$c_1 h_L^\alpha = c_1 \left(h_0s^{-L}\right)^\alpha \leq \frac{\varepsilon}{2},$$

or equivalently letting $L = \left\lceil \frac{\log(2c_1 h_0^\alpha \varepsilon^{-1})}{\alpha \log(s)} \right\rceil$, which implies

$$\frac{\log(2c_1 h_0^\alpha \varepsilon^{-1})}{\alpha \log(s)} \leq L < \frac{\log(2c_1 h_0^\alpha \varepsilon^{-1})}{\alpha \log(s)} + 1 = \frac{\log(2c_1 h_0^\alpha \varepsilon^{-1})}{\alpha \log(s)}.$$ (63)
As a direct consequence, 
\[ h_0(2c_1)^\theta \rho^\theta \leq s^\theta < sh_0(2c_1)^\theta \rho^{\theta}. \]

(64)

We now show that choices (40) and (47) of sample sizes have the advertised computational cost. As before, we first consider the multilevel sampling scheme for which the sampling error contains no logarithmic term. Recall that the total cost (41) associated with formula (40) satisfies

\[ \sum_{s=0}^L C_l M_l = (2c_3 \rho^{-1})^{\frac{\theta}{\rho}} \left( \sum_{s=0}^L (C_l^\theta \varphi(\Delta u_s))^{\frac{\theta}{\rho}} \right)^{\frac{\rho-1}{\rho}}. \]

Seeing that the sum \( \sum_{s=0}^L (C_l^\theta \varphi(\Delta u_s))^{\frac{\theta}{\rho}} \) appears frequently in sequel, it is useful to first estimate its upper bound in terms of \( \varepsilon \). Under Assumptions (A2) and (A4),

\[ \sum_{s=0}^L (C_l^\theta \varphi(\Delta u_s))^{\frac{\theta}{\rho}} \leq (c_2 \varepsilon c_1 h_0^\theta)^\frac{\theta}{\rho} \sum_{s=0}^L \frac{\rho-1}{\rho} - \frac{\rho-1}{\rho} \sum_{s=0}^L \frac{\rho-1}{\rho} = (c_2 \varepsilon c_1 h_0^\theta)^\frac{\theta}{\rho} \sum_{s=0}^L \frac{\rho-1}{\rho}. \]

(65)

The upper bound for the geometric series \( \sum_{s=0}^L \frac{\rho-1}{\rho} \) depends on the sign of the quantity \( \beta - \gamma \mu \) and we therefore treat each case separately.

**Case 1:** \( \beta < \gamma \mu \). When the growth in the cost outweighs the decay of the correction terms, then the terms \( s^{-\frac{\rho-1}{\rho}} \) are increasing with \( \ell \). We can now use inequality (64) to bound the geometric series by

\[ \sum_{s=0}^L s^{-\frac{\rho-1}{\rho}} = \frac{s^{\frac{\rho-1}{\rho}} - 1}{s^{\frac{\rho-1}{\rho}} - 1} \leq (2c_1 h_0^\theta \rho^{-1})^{\frac{\theta}{\rho}} \sum_{s=0}^L \frac{\rho-1}{\rho} \leq (2c_1 h_0^\theta \rho^{-1})^{\frac{\theta}{\rho}}. \]

(66)

**Case 2:** \( \beta = \gamma \mu \). In this case

\[ \sum_{s=0}^L s^{-\frac{\rho-1}{\rho}} = (L + 1) \leq \frac{1}{a \log(s)} \log(2c_1 (h_0 s^2)^a) \rho \quad \leq \frac{1}{a \log(s)} \log(2c_1 (h_0 s^2)^a) \rho \quad \leq \frac{1}{a \log(s)} \log(2c_1 (h_0 s^2)^a) \rho, \]

(67)

since \( \varepsilon < \frac{1}{\rho} \).

**Case 3:** \( \beta > \gamma \mu \). In this case the terms \( s^{-\frac{\rho-1}{\rho}} \) are decreasing with \( \ell \), and therefore the geomet-
Next, we consider the total cost when the sample sizes are chosen according to (47), i.e.

Substituting (69) into the total cost (41) now yields

\[
\sum_{\ell=0}^{L} \left( C_{\ell} \right) \leq \frac{1 - s^{-\frac{C_{0}}{s_{0}M \alpha}}}{1 - s^{-\frac{C_{0}}{s_{0}M \alpha}}},
\]

(68)

Combining inequality (68) with estimates (66), (67) and (69) respectively, we obtain

\[
\sum_{\ell=0}^{L} \left( C_{\ell} \psi(\Delta V_{\ell}) \right) \leq \begin{cases} 
\frac{1}{\bar{d}_{1}} \epsilon^{-\frac{C_{0}}{s_{0}M \alpha}}, & \text{if } \beta < \gamma \mu_{2} \\
\frac{1}{\bar{d}_{2}} \log(\epsilon^{-1}), & \text{if } \beta = \gamma \mu_{2} \\
\frac{1}{\bar{d}_{3}}, & \text{if } \beta > \gamma \mu_{2}
\end{cases}
\]

(69)

where

\[
\bar{d}_{1} = (c_{2} c_{4} \delta^{\mu_{2}}) \epsilon^{-\frac{C_{0}}{s_{0}M \alpha}} \left( \frac{2c_{1}h_{0}^{\mu_{2}}}{s_{0}M} \right)
\]

\[
\bar{d}_{2} = (c_{2} c_{4} \delta^{\mu_{2}}) \epsilon^{-\frac{C_{0}}{s_{0}M \alpha}} \left( \frac{1 + \log(2c_{1}h_{0}s_{0}^{2})}{\alpha \log(s)} \right)
\]

\[
\bar{d}_{3} = (c_{2} c_{4} \delta^{\mu_{2}}) \epsilon^{-\frac{C_{0}}{s_{0}M \alpha}} \left( \frac{1}{1 - s^{-\frac{C_{0}}{s_{0}M \alpha}}} \right)
\]

Substituting (69) into the total cost (41) now yields

\[
\sum_{\ell=0}^{L} C_{\ell} M_{l} \leq \begin{cases} 
\frac{(2c_{3} \bar{d}_{1}^{\mu_{2}}) \epsilon^{-\frac{C_{0}}{s_{0}M \alpha}}}{\delta^{\mu_{2}}}, & \text{if } \beta < \gamma \mu_{2} \\
\frac{(2c_{3} \bar{d}_{2}^{\mu_{2}}) \epsilon^{-\frac{C_{0}}{s_{0}M \alpha}}}{\delta^{\mu_{2}} \log(\epsilon^{-1})}, & \text{if } \beta = \gamma \mu_{2} \\
\frac{(2c_{3} \bar{d}_{3}^{\mu_{2}}) \epsilon^{-\frac{C_{0}}{s_{0}M \alpha}}}{\delta^{\mu_{2}}}, & \text{if } \beta > \gamma \mu_{2}
\end{cases}
\]

(70)

Next, we consider the total cost when the sample sizes are chosen according to (47), i.e.

\[
\sum_{\ell=0}^{L} M_{l} C_{\ell} \leq \left( \frac{C_{3}}{K_{1}} \right)^{\frac{1}{\mu_{2}}} \lambda^{\frac{\mu_{2}}{\delta^{\mu_{2}}}} \sum_{\ell=0}^{L} \left( C_{\ell} \psi(\Delta V_{\ell}) \right)^{\frac{1}{\mu_{2}}} \log \left( \frac{K_{1} C_{\ell}}{(\lambda C_{\ell})^{\frac{1}{\mu_{2}}}} \right) + C_{\ell}
\]

The sum \( \sum_{\ell=0}^{L} C_{\ell} \) can readily be shown to have an upper bound similar to (55). In fact, under Assumption (A2)

\[
\sum_{\ell=0}^{L} C_{\ell} \leq c_{2} h_{0}^{\mu_{2}} \sum_{\ell=0}^{L} s^{\mu_{2}} \leq (2c_{1}h_{0}^{\mu_{2}})^{\frac{1}{\mu_{2}}} \epsilon^{-\frac{\gamma}{\mu_{2}}} < (2c_{1}h_{0}^{\mu_{2}})^{\frac{1}{\mu_{2}}} \epsilon^{-\frac{\gamma}{\mu_{2}}},
\]

(71)
since \( \alpha < \mu_2 \gamma \). Consider the log term

\[
\log \left( \frac{K_1 C_\ell}{\lambda C_3 \varphi(\Delta u_\ell)} \right)
\]

Since the computational cost at the lowest spatial refinement level satisfies \( C_0 \leq C_\ell \) for \( \ell > 0 \) it follows by virtue of Assumption (A2) that

\[
\frac{\varphi(\Delta u_\ell)}{C_\ell} \leq \frac{c_2 h_\ell^{\beta}}{C_0} \leq \frac{c_2 h_0^{\beta}}{C_0}.
\]

Moreover, according to (69),

\[
\sum_{\ell' = 0}^{\ell} (C_{\ell'} \| \Delta u_{\ell'} \|)^{\frac{\mu_2}{\mu_1}} \leq \max_{i=1,2,3} \{ \tilde{d}_i \} e^{-\max_{i=1,2,3} \frac{\mu_2}{\mu_1}}.
\]

Combining (74) with (73) in (72) now yields

\[
\log \left( \frac{C_\ell}{\lambda C_3 \varphi(\Delta u_\ell)} \right)^{\frac{\tilde{d}_i}{\mu_2}} \leq \log(K_2 e^{-K_1})^{\frac{\mu_2}{\alpha}} \leq (\log(K_2) + K_3)^{\frac{\mu_2}{\alpha}} \log(e^{-1})^{\frac{\mu_2}{\alpha}},
\]

where

\[
K_2 = K_1^{-1} C_0^{-1} \gamma^{1/2} c_2^{1/2} c_3^{\mu_2/\mu_1} \max_{i=1,2,3} \{ \tilde{d}_i \}^{\frac{\mu_2}{\mu_1}},
\]

and

\[
K_3 = \left( \max \{ 1, \frac{\gamma \mu_2 - \beta}{\alpha (\mu_2 + 1)} \} \frac{\mu_2 + 1}{\mu_2} \right)
\]

Incorporating the upper bounds (69), (71) and (75) into the total cost (50) and using expression
Indeed it can be shown that the covariance function
\[ \text{univariate random field defined at} \]
\[ \text{For short correlation lengths, finite noise approximations of} \]
diagonal algorithms to estimate the spatially varying mean of the solution to the elliptic equation (8) with (46) for \( \lambda \), we finally get
\[
\sum_{l=0}^{\infty} \mathcal{C}_l \mathcal{M}_l \leq \left( \frac{c_3}{K_1} \right)^{1/\nu} (\log(K_2) + K_3)^{d_1} \log(e^{-1}) \sum_{l=0}^{\infty} \mathcal{C}_l \mathcal{M}_l \leq \sum_{l=0}^{\infty} \mathcal{C}_l \mathcal{M}_l + \sum_{l=0}^{\infty} \mathcal{C}_l \mathcal{M}_l \\
\leq \left\{ \begin{array}{ll}
d_1 e^{-\frac{1}{\nu} \log(e^{-1}) \frac{d_1}{2}}, & \text{if } \beta < \gamma \mu_2 \\
d_2 e^{-\frac{1}{\nu} \log(e^{-1}) \frac{d_2}{2}}, & \text{if } \beta = \gamma \mu_2 \\
d_3 e^{-\frac{1}{\nu} \log(e^{-1}) \frac{d_3}{2}}, & \text{if } \beta > \gamma \mu_2 \\
\end{array} \right.
\]
\[ \text{where } d_i = \frac{1}{\nu} K_1^{\frac{1}{\nu}} (\log(K_2) + K_3)^{\frac{d_i}{2}} e^{\frac{d_i}{2}} + (2 \mathcal{C}_1 \mathcal{M}_0)^{\frac{d_i}{2}} \text{ for } i = 1, 2, 3. \]

5. Numerical Examples

This section discusses the numerical implementation of the multilevel sparse grid algorithm described in the previous sections. We apply both the multilevel Monte Carlo and sparse grid algorithms to estimate the spatially varying mean of the solution to the elliptic equation (8) with a random diffusion coefficient on either the unit interval, i.e. \( D = [0, 1] \) or the unit square, i.e. \( D = [0, 1]^2 \). For both these spatial domains, we choose the diffusion coefficient \( q \) to be the univariate random field defined at \( x_1 \in [0, 1] \) by
\[
\log(a(x_1, \omega) - 0.5) = 1 + \left( \frac{\sqrt{\pi} L}{2} \right)^{1/2} Y_1(\omega) + \sum_{n=2}^{\infty} b_n(x_1) Y_n(\omega),
\]
where
\[
b_n(x_1) := \left( \frac{\sqrt{\pi} L}{2} \right)^{1/2} \exp\left( -\frac{(\log(\frac{n}{q} \sqrt{L}))^2}{8} \right) \frac{\sin\left( \frac{L \pi n}{L} \right)}{\cos\left( \frac{L \pi n}{L} \right)} \text{ if } n \text{ is even},
\]
\[
b_n(x_1) := \left( \frac{\sqrt{\pi} L}{2} \right)^{1/2} \exp\left( -\frac{(\log(\frac{n}{q} \sqrt{L}))^2}{8} \right) \frac{\cos\left( \frac{L \pi n}{L} \right)}{\sin\left( \frac{L \pi n}{L} \right)} \text{ if } n \text{ is odd},
\]
and the random variables \( \{ Y_n \}_{n=1}^{\infty} \) are independent and uniformly distributed over the interval \([ -\sqrt{3}, \sqrt{3} ] \). The parameter \( L \) relates to the correlation length of the field \( \log(q(x, \omega) - 0.5) \). Indeed it can be shown that the covariance function
\[
\text{Cov}[\log(a - 0.5)(x_1, x_1')] = \exp\left( \frac{-(x_1 - x_1')^2}{L^2} \right).
\]
For short correlation lengths, finite noise approximations of \( q \) require a large number of terms to accurately represent its correlation structure, leading not only to a high stochastic dimension, but also to the presence of fine scale oscillations that can only be resolved with sufficiently fine meshes (see [13]). Here we do not consider the effect of this truncation error, and take \( L = 0.25 \) and \( N = 5 \). We also let the deterministic forcing term \( f \) be given by \( f(x_1) = \cos(x_1) \) when \( D = [0, 1] \), and \( f(x_1, x_2) = \cos(x_1) \sin(x_2) \), when \( D = [0, 1]^2 \). The parameters \( f \) and \( q \) readily satisfy the smoothness conditions made in Assumptions 2 and 3 justifying the use of sparse grids.
and were in fact used in [16] to show the competitive convergence rate of sparse grid methods vis-à-vis Monte Carlo sampling and stochastic finite elements.

We solve each realization of the system using the finite element method with continuous piecewise polynomial basis functions and computational cost per solve was measured in CPU time. We obtained estimates for the spatial error through the spatial $L^2$ norms of the correction terms and for the sparse grid quadrature error by comparing successive sparse grid approximations $I_M[v]$ in the spatial $L^2$ norm. Since the convergence rates of sparse grid stochastic collocation methods depend on quantities that can not readily be computed \textit{a priori}, such as the radii $\tau_n$ of the regions of analyticity, they must be estimated during the execution of the program, unlike that of the Monte Carlo method ($\mu_2 = \frac{1}{2}$). We achieve and update this estimate by generating an initial sample on the coarsest level as well as after each spatial refinement step, before computing the optimal sample sizes. An overly conservative initial sample size will generate more sample paths than are necessary, especially when the sampling scheme has a fast convergence rate, while a sample size that is too small may lead to inaccurate diagnostic parameters, both of which have a detrimental effect on the efficiency of the algorithm. To mitigate this risk, we begin with a relatively large initial sample size on the coarsest level and reduce it gradually as our confidence in the estimated convergence rate improves.

Example 1 (1D). Let $D = [0, 1]$ with an initial mesh of uniform subintervals of length $h = 1/8$. We use a tolerance level $\varepsilon = 10^{-3}$ and refine the mesh by scaling $h$ at each step by the factor $s = 4$. Figure 1 plots the $\varepsilon$-cost for single- and multi-level versions of both Monte Carlo sampling and sparse grid stochastic collocation, based on different spatial refinement levels. As expected, the sparse grid stochastic collocation method is more efficient than Monte Carlo sampling and in both cases the multilevel algorithm achieves a considerable speed-up. For this example, four spatial mesh refinements are required to obtain a spatial error within tolerance (see Figure 2a).
Figure 1: The total $\varepsilon$-cost of the single- and multilevel Monte Carlo (slmc, mlmc) and sparse grid (slsg, mlsg, mlsg bin) methods. The dataset 'mlsg' represents the computed optimal sample sizes, while 'mlsg bin' refers to the binned sample sizes used to generate the actual multilevel estimate.

From our analysis (Theorem 1) it would seem that a faster spatial convergence rate, i.e. a higher value of $\alpha$ would improve the overall efficiency. Figure shows this to be the case for our example. Indeed not only are fewer refinement steps necessary for higher order polynomial approximation, but the computational effort also decreases.
Figure 3: The effect of using a higher order finite element method on the efficiency of the multilevel algorithm.

In order to investigate the effect of the refinement parameter $s$ and the number of spatial refinement steps needed on the algorithm’s efficiency, we repeated Example 1 using linear basis functions, but with different values of $s$, ranging from $s = 2, 4, 6, 8, 10$ to $s = 160$. We computed the extreme value $s = 160$, based on diagnostic information from previous examples by determining the mesh width $h$ for which the spatial error is within tolerance, so that with $s = 160$ only one refinement step is necessary. We also used the previous, more accurate convergence rates to determine the optimal sample sizes. In other words, the case $s = 160$ is unrealistic but was used to shed some light on the effect that the number of refinement steps has on the overall efficiency.
The results, as summarized in Figure 4, are not conclusive. It seems (see Figure 4b) that there is an optimal value for $s$, in this case $s = 6$, for which the computational effort is minimal. More moderate refinement strategies may lead to a needlessly many levels and hence too many unnecessary samples, while those that are overly aggressive might overshoot the mesh size $h$ required by the tolerance level (see Figure 4a), thereby incurring a needlessly high cost. These, however cannot be the only determinants of efficiency, since the value $s = 160$, giving precisely the right $h$, would then be expected to outperform the others. In other words, the number of spatial refinement models also seems to have an influence on the overall efficiency of the algorithm. More work is needed to untangle the effect of the mesh refinement strategy on the $\varepsilon$-cost of the algorithm.

Example 2 (2D). Consider the spatial domain $D = [0, 1]^2$ subdivided by uniform triangulation with mesh width $h = 0.25$. Here we use the same tolerance level as before, i.e. $\varepsilon = 10^{-3}$ and refine the mesh at each step by dyadic subdivision, i.e. $s = 2$. The results are comparable to those in Example 1. The sparse grid method outperforms the Monte Carlo sampling scheme in both the single- and multilevel cases, although the multilevel Monte Carlo method is more efficient than the single level sparse grid method in this case. The degrees of freedom of the sample deterministic systems ranged from 64 to 16641 and in fact the maximal number of refinement steps were reached before the spatial error estimate was within tolerance. At such high refinement levels, it is not only the deterministic system solve, but also the assembly and interpolation operations that contribute significantly to the overhead. On the other hand, there is a wealth of information available from samples already generated, which could potentially be incorporated into the assembly and solution of a given system realization, thus providing a much needed speed-up.
Multilevel sampling methods offer an improvement on the efficiency of single level methods without loosing any of their salient features, such as parallel implementation, nestedness, or non-intrusiveness. In this paper we have shown that the multilevel Monte Carlo algorithm developed in [11] can readily be extended to interpolation-based sampling schemes (such as sparse grid stochastic collocation) leading to an even greater efficiency in certain cases. Despite the technical difficulties in proving that the multilevel algorithm improves the computational complexity, this method is surprisingly straightforward to implement if the errors and convergence rates are estimated numerically. This supports the claim that the multilevel algorithm can be used as a wrapper, coordinating the spatial refinement with the quadrature level. An area of future work would be to investigate this claim in the case of adaptive sampling schemes. Furthermore, it is not yet entirely clear how the spatial refinement strategy effects the overall performance of the algorithm, although it was seen in to have a considerable influence. Apart from improving efficiency, multilevel methods strategically record useful information that can be harnessed to further improve computation.

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Mesh Width, $h$

Cost per Sample [sec]

- $mc$
- $sg$