Quasi-Monte Carlo finite element approximation of the Navier–Stokes equations with log-normal initial data

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Abstract

In this work, we investigate the numerical approximation of the Navier–Stokes equations on a bounded polygonal domain in $\mathbb{R}^2$, where the initial condition is modeled by a log-normal random field. We propose a novel numerical scheme to compute the expected value of linear functionals of the solution to the Navier–Stokes equations. The scheme is based on the finite element discretization in space, backward Euler method in time, truncated Karhunen–Loève expansion for realizing the random initial condition, and lattice-based quasi-Monte Carlo (QMC) for estimating the expected values over the parameter space (i.e., randomly-shifted lattice rules for the integration over a high-dimensional hypercube). We present a rigorous error analysis of the numerical scheme, including bounds on the mean squared error, and especially establish that the QMC converges optimally at an almost-linear rate with the constant independent of the dimension of integration. To the best of our knowledge, this represents the first rigorous theoretical analysis of QMC sampling strategy for nonlinear problems.

Keywords: quasi-Monte Carlo method, finite element method, uncertainty quantification, Navier–Stokes equations, random initial data, log-normal random field, Karhunen–Loève expansion

Mathematics Subject Classification: 65D40, 65D32, 65N30, 76D05
1 Introduction

Uncertainty in the input data of mathematical models has received much recent attention due to its importance in various applications. The uncertainty can arise from different sources, e.g., coefficients, boundary conditions, initial conditions, and external forces. The impact of uncertainty on various quantities of interest sheds valuable insights into the inherent variability of diverse physical and engineering problems.

To describe and analyze uncertainty, probability theory offers a flexible framework where uncertain inputs are treated as random fields, and it is especially useful in characterizing the randomness associated with physical quantities of a given system.

In this work, we investigate the incompressible Navier-Stokes equations with random initial data. Let $D \subset \mathbb{R}^2$ be a bounded convex polygonal domain. Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space, where $\Omega$ is a sample space consisting of all possible outcomes, $\mathcal{F} \subset 2^\Omega$ a $\sigma$-algebra, and $\mathbb{P} : \mathcal{F} \to [0, 1]$ a probability function. Consider the following initial-boundary value problem: find a random velocity field $u : [0, T] \times D \times \Omega \to \mathbb{R}^2$ and a random pressure field $p : [0, T] \times D \times \Omega \to \mathbb{R}$ such that the following equations hold $\mathbb{P}$-almost surely (a.s.):

\begin{align}
\partial_t u + (u \cdot \nabla) u - \nabla p &= 0, \quad \text{in } [0, T] \times D \times \Omega, \\
\text{div } u &= 0, \quad \text{in } [0, T] \times D \times \Omega,
\end{align}

where the symbols $\nabla$ and $\Delta$ denote differential operators with respect to the spatial variable $x \in D$, while $\partial_t$ denotes the time derivative. The system is subject to the homogeneous boundary condition and random initial condition:

\begin{align}
u(t, x, \omega) &= 0, \quad \text{on } (0, T] \times \partial D \times \Omega, \\
u(0, x, \omega) &= u^0(x, \omega), \quad \text{in } D \times \Omega.
\end{align}

In this work, we consider the following initial random field $u^0(x, \omega) : D \times \Omega \to \mathbb{R}$:

\begin{equation}
u^0(x, \omega) = \nabla^\perp \exp(Z(x, \omega)) = \left(-\partial_{x_2} \exp(Z(x, \omega)), \partial_{x_1} \exp(Z(x, \omega))\right), \end{equation}

where $Z(\cdot, \cdot)$ is a centered Gaussian random field. The choice (5) ensures that the initial condition $u^0$ is divergence-free, i.e., $\text{div } u^0(x, \omega) = 0$ in $D \times \Omega$. The quantity of interest is the expected value of $\mathcal{G}(u)$ for any linear functional $\mathcal{G} \in (L^2(D))^2$, associated with the solution $u$ of problem (1)-(5), where $(L^2(D))^2$ refers to the dual space of $L^2(D)^2$.

We shall develop and analyze a novel algorithm for computing the expected value $\mathbb{E}[\mathcal{G}(u)]$. The proposed scheme consists of three steps. The first step involves solving problem (1)-(4) for a fixed $\omega \in \Omega$ using a fully-discrete finite element method (FEM) scheme, based on backward Euler in time (with a time step size $\tau$) and conforming finite element approximation on a regular mesh of the domain $D$ (with a mesh size $h$). We denote the finite element solution at time step $J$ by $u^J_h$. The second step involves truncating the Karhunen-Loève (KL) expansion [1, 2] of the random initial data $u^0(x, \omega)$ in (5), which parameterizes $u^0$ by a countable number of random variables, cf. (10) below: We truncate the infinite series in (10) with a sum with $s$
terms, \( s \in \mathbb{N} \), and obtain a truncated problem with a finite-dimensional random vector \( y = (y_1(\omega), \ldots, y_s(\omega)) \). We denote by \( u_{s,h}^J \) the FEM solution of the truncated problem. In the third step, we approximate the quantity of interest \( E[G(u(t_J))] \) by the expected value \( E[G(u_{s,h}(\omega))] \), and compute the integral using quasi-Monte Carlo (QMC) methods [3–5]. Let \( \varphi(y) = \exp(-y^2/2)/\sqrt{2\pi} \) be the probability density function (PDF) of the standard normal distribution, and \( \Phi_s \) the cumulative distribution function (CDF) of the standard normal random vector of length \( s \in \mathbb{N} \), and \( \Phi_s^{-1}(v) \) its inverse for \( v \in [0,1]^s \). Then with \( F_{s,h}^J(y) = G(u_{s,h}(\cdot, y)) \),

\[
E[G(u_{s,h}^J)] = \int_{\mathbb{R}^s} G(u_{s,h}^J(\cdot, y)) \prod_{i=1}^s \varphi(y_i) \, dy = \mathbb{E}[F_{s,h}^J] = \int_{(0,1)^s} F_{s,h}^J(\Phi_s^{-1}(v)) \, dv. \tag{6}
\]

To approximate (6), we use a QMC quadrature rule, i.e., randomly-shifted lattice rule (RSLRs):

\[
\mathcal{Q}_{s,N}(F_{s,h}^J; \Delta) := \frac{1}{N} \sum_{i=1}^N F_{s,h}^J(\Phi_s^{-1}\left(\frac{iz}{N} + \Delta\right)) ,
\]

where \( z \in \mathbb{N}^s \) is a generating vector, \( \Delta \) is a random shift uniformly distributed over \([0,1]^s\), and the function \( \text{frac}(\cdot) \) takes the fractional part of its argument.

The design and analysis of QMC methods for linear PDEs with random coefficients, where the QMC methods are utilized to estimate the expected values of linear functionals of the exact or approximate solution from the PDEs, has been well investigated in the past ten years [34, 35, 40]. The expected values can be transformed into an infinite or high dimensional integral over the parameter domain, which corresponds to the randomness induced by the random coefficient. A proper function space for a given integrand should be designed to guarantee this high-dimensional integration problem is tractable. The “standard” function spaces in the QMC analysis are weighted Sobolev spaces on \((0,1)^s\), which consists of functions with square-integrable mixed first derivatives. If the integrand lies in a suitable weighted Sobolev space, then RSLRs can be constructed so as to (nearly) achieve the convergence rate \( O(n^{-1}) \); see [21–25] and recent surveys [26, 27].

In this work, we provide a thorough analysis of the numerical approximation \( \mathcal{Q}_{s,N}(F_{s,h}^J; \Delta) \). This is achieved by decomposing the error into the finite element error, the error due to KL truncation, and the error due to the QMC quadrature. In Theorem 14, we establish a bound on the root-mean-square error at each time level \( J \), i.e.,

\[
(\mathbb{E}[G(u(t_J))] - \mathbb{E}[\mathcal{Q}_{s,N}(F_{s,h}^J; \Delta)])^2 \right)^{1/2} ,
\]

where \( \mathbb{E}[\cdot] \) denotes taking expectation with respect to the random shift \( \Delta \). The main technical challenge in the analysis is to bound the mixed derivatives of the velocity field with respect to the stochastic variable in suitable weighted Sobolev norms. This issue is highly challenging due to the non-linearity of the mathematical model. These estimates are established in Theorem 8, which allows deriving an error estimate for the QMC sampling strategy applied to the Navier–Stokes equations. To the best of the authors’ knowledge, this work represents the first rigorous analysis of quasi-Monte Carlo (QMC) methods for nonlinear PDEs. This contribution advances the use of QMC methods in the context of nonlinear PDEs.
The rest of the paper is organized as follows. In Section 2, we describe the variational formulation of the Navier–Stokes equations and its well-posedness, and give assumptions on the initial data $u^0$. In Section 3, we give a fully discrete FEM approximation and discuss its convergence rate. In Section 4, we analyze the truncated KL expansion. In Section 5, we describe the QMC quadrature rule for approximating the integral and derive an error bound. To complement the theoretical findings, we present several numerical experiments in Section 6. In Section 7, we give concluding remarks. In the appendix, we collect several useful inequalities.

We conclude with useful function spaces. For $m \geq 0$ and $1 \leq p \leq \infty$, we denote by $L^p(D)$ and $W^{m,p}(D)$ the standard Lebesgue and Sobolev spaces, and when $p = 2$, we write $H^m(D) := W^{m,2}(D)$. We denote by $H^1_0(D)$ the space of functions in $H^1(D)$ with zero trace on $\partial D$ and by $C^\infty_0(D)$ the space of $C^\infty$ functions with compact support in $D$. The notation $X(D)^d$ denotes the $d$-fold product space of $X(D)$, and $a \cdot b$ denotes the scalar product of two vectors $a$ and $b$. Also, $C$ denotes a generic positive constant, which may change at each appearance, and $A \lesssim B$ means that there exists $C > 0$ such that $A \leq CB$.

## 2 Weak formulation of the parametric problem

First we define the following functional spaces that are frequently used in the study of incompressible fluid flow:

$$
V = \{ u \in C^\infty_0(D)^2 : \text{div} u = 0 \}, \quad V = H^1_0(D)^2, \quad H = L^2(D)^2.
$$

The space $H$ is a Hilbert space with the $L^2(D)$ inner product $(\cdot, \cdot)$, and the space $V$ is equipped with the scalar product $a(u, v) = \int_D \nabla u : \nabla v \, dx$. Further, we define a trilinear form $B : V \times V \times V \rightarrow \mathbb{R}$ by

$$
B[u, v, w] = \frac{1}{2} \int_D ((u \cdot \nabla)v) \cdot w - ((u \cdot \nabla)w) \cdot v \, dx. \quad (7)
$$

This modified convective term conserves the skew symmetry of discrete divergence, cf. (18) below. Note that $B[\cdot, \cdot, \cdot]$ coincides with the trilinear form associated with the convection term in (1) for pointwise divergence-free functions.

We have the following well-posedness of problem (1)-(4) in the 2D case [6].

**Theorem 1.** For any given $u^0 \in H$, there exists a unique $u \in L^\infty(0,T;H) \cap L^2(0,T;V)$ such that

$$
\begin{align*}
(\partial_t u, v) + B[u, u, v] + a(u, v) &= 0, \quad \forall v \in V, \\
u(0) &= u^0. 
\end{align*}
$$

Furthermore, the following energy estimate holds

$$
\sup_{0 < t < T} \| u(t) \|_{L^2(D)}^2 + \frac{2}{T} \int_0^T \| \nabla u(\tau) \|_{L^2(D)}^2 \, d\tau \leq \| u^0 \|_{L^2(D)}^2. 
$$

4
It is direct to show that $\partial_t u \in L^2(0, T; V')$, which implies $u \in C([0, T]; H)$. Thus the identity $u(0) = u^0$ in (8) makes sense. We restrict our discussion to the 2D case for which the uniqueness of the weak solution to (8) is known. The analysis can be extended to the 3D case if the uniqueness holds. This is known only under more restrictive assumptions; see e.g., [6] for local well-posedness under Serrin condition.

The weak formulation (8) motivates the deterministic variational formulation of problem (1)-(4). Following standard practice [1, 2], we assume that the given Gaussian random field $Z(\cdot, \cdot)$ in (5) can be parameterized by Karhunen-Loève (KL) expansion:

$$Z(x, \omega) = \sum_{j=1}^{\infty} \sqrt{\mu_j} \xi_j(x) y_j(\omega), \quad (x, \omega) \in D \times \Omega, \quad (10)$$

where $\{y_j\}_{j \geq 1}$ is a sequence of independently and identically distributed (i.i.d.) random variables following the standard normal distribution $\mathcal{N}(0, 1)$. Let the sequence $\{(\mu_j, \xi_j)\}_{j \geq 1}$ be the eigenpairs of the covariance operator:

$$\mathcal{C}v(x) := \int_D c(x, x') v(x') \, dx'.$$ (11)

Here, the kernel $c(\cdot, \cdot)$ denotes the covariance function of $Z(\cdot, \cdot)$ and is defined by $c(x, x') = \mathbb{E}[Z(x, \cdot)Z(x', \cdot)]$ for any $x, x' \in D$. The integral operator $\mathcal{C}$ is self-adjoint and compact from $L^2(D)$ into $L^2(D)$. The non-negative eigenvalues, $\|c(x, x')\|_{L^2(D \times D)} \geq \mu_1 \geq \mu_2 \geq \cdots \geq 0$, satisfy $\sum_{j=1}^{\infty} \mu_j = \int_D \text{Var}(Z)(x) \, dx$, and the eigenfunctions are orthonormal in $L^2(D)$, i.e., $\int_D \xi_j(x) \xi_k(x) \, dx = \delta_{jk}$.

It follows from (5) and (10) that the initial condition $u^0(\cdot, \omega)$ can be parametrized by an infinite-dimensional vector $y(\omega) = (y_1(\omega), y_2(\omega), \cdots) \in \mathbb{R}^\infty$ (of i.i.d. Gaussian random variables $y_j \sim \mathcal{N}(0, 1)$). The law of $y$ is defined on the probability space $(\mathbb{R}^\infty, \mathcal{B}(\mathbb{R}^\infty), \mu_G)$, where $\mathcal{B}(\mathbb{R}^\infty)$ is the Borel $\sigma$-algebra on $\mathbb{R}^\infty$ and $\mu_G$ denotes the product Gaussian measure [7]: $\mu_G = \bigotimes_{j=1}^{\infty} \mathcal{N}(0, 1)$.

Throughout, we make the following regularity assumption on $Z(x, \omega)$.

**Assumption 2.** For some $k > 3$, $Z(x, \omega) \in L^2(\Omega; H^k(D))$.

Under Assumption 2, the eigenvalues $\mu_j$ satisfy [8]

$$\mu_j \lesssim j^{-k-1} \text{ for } j \in \mathbb{N} \text{ sufficiently large.} \quad (12)$$

Under Assumption 2, we have $\|\xi_j\|_{H^\theta(D)} \lesssim j^{\frac{k+1}{2} \theta}$ for any $0 \leq \theta \leq 1$ [8]. This and Sobolev embedding directly imply

$$\|\xi_j\|_{C(\partial D)} \lesssim j \quad \text{and} \quad \|\nabla \xi_j\|_{C(\partial D)} \lesssim j^{3/2} \text{ for } j \in \mathbb{N} \text{ sufficiently large.} \quad (13)$$

We define the sequence $b = \{b_j\}_{j\geq 1}$ by

$$b_j := \sqrt{\mu_j} \|\xi_j\|_{C(\partial D)}, \quad j \geq 1,$$ (14)
For the QMC analysis in Section 5, we make the following assumption. If \( k > \frac{3}{p} \), then Assumption 2 and (12) imply Assumption 3.

**Assumption 3.** There exists some \( p \in (0, 1] \) such that \( \sum_{j \geq 1} b_j < \infty \).

Next, we define the following admissible parameter set

\[
U_b := \left\{ y \in \mathbb{R}^\infty : \sum_{j \geq 1} b_j |y_j| < \infty \right\} \subset \mathbb{R}^\infty.
\]

Note that the set \( U_b \subset \mathbb{R}^\infty \) is not a product of subsets of \( \mathbb{R} \). However, if Assumption 3 hold for some \( 0 < p < 1 \), the set is \( \overline{\mu}_G \)-measurable and of full Gaussian measure, i.e., \( \overline{\mu}_G(U_b) = 1 \) [9, Lemma 2.28]. Since \( \overline{\mu}_G(U_b) = 1 \), we can use \( U_b \) as the parameter space instead of \( \mathbb{R}^\infty \). Note that \( U_b \) is not a product domain. But we can define a product measure, e.g., \( \overline{\mu}_G \) on \( U_b \) by restriction. Thus, we can identify the random initial condition \( u^0(x, \omega) \) with its parametric representation \( u^0(x, y(\omega)) \): for each \( y \in U_b \), we define the deterministic initial condition by

\[
\begin{align*}
\dot{\mathbf{u}}^0(x, y) &= -\partial_{x_2} \exp \left( \sum_{j=1}^{\infty} \sqrt{\mu_j} \xi_j(x) y_j \right), \\
\partial_{x_1} \exp \left( \sum_{j=1}^{\infty} \sqrt{\mu_j} \xi_j(x) y_j \right).
\end{align*}
\]

(15)

Accordingly, we consider the following deterministic and parametric variational formulation of problem (1)–(4): For each \( y \in U_b \), find \( u(y) \in V \) satisfying

\[
\begin{align*}
(\partial_t u(y), v) + B[u(y), u(y), v] + a(u(y), v) &= 0, \quad \forall v \in V, \\
u(0, y) &= u^0(y).
\end{align*}
\]

(16)

Note that \( u^0(y) \in H \) for each \( y \in U_b \), due to Assumption 2. This and Theorem 1 imply that the solution \( u(y) \) is uniquely determined for each \( y \in U_b \).

### 3 Finite element approximation

We employ the implicit conforming Galerkin FEM approximation for the variational formulation (16) of the Navier–Stokes system. Let \( T_h \) be a shape-regular partition of the domain \( D \) with a mesh size \( h \). We define conforming FEM spaces for the velocity \( H_h \subset H_0^1(D)^2 \) and the pressure \( L_h \subset L_0^2(D) \) by

\[
\begin{align*}
H_h &= \{ \mathbf{W} \in C(\overline{D})^2 : \mathbf{W}|_K \in P_i(K)^2, \; \forall K \in T_h \text{ and } \mathbf{W}|_{\partial D} = 0 \}, \\
L_h &= \{ \Pi \in L_0^2(D) : \Pi|_K \in P_j(K), \; \forall K \in T_h \},
\end{align*}
\]

where \( P_i(K) \) denotes the space of polynomials of degree \( i \) on the triangle \( K \in T_h \). The FEM spaces \( H_h \) and \( L_h \) are assumed to satisfy the discrete inf-sup condition:

\[
\|q_h\|_{L_2(D)} \leq C \sup_{v_h \in H_h \setminus \{0\}} \frac{(\nabla \cdot v_h, q_h)}{\|\nabla v_h\|_{L_2(D)}}, \quad \forall q_h \in L_h,
\]

(17)
where the constant $C > 0$ is independent of $h$. This condition holds for several finite element spaces, e.g., Taylor-Hood element or MINI element \cite{10}. Also we define a discrete divergence-free subspace of $H_h$ by

$$V_h := \{ v_h \in H_h : (\nabla \cdot v_h, q_h) = 0, \ \forall q_h \in Q_h \}. \quad (18)$$

Given \( \ell \in \mathbb{N} \), we divide the interval $[0, T]$ into a uniform grid $0 = t_0 < t_1 < \cdots < t_\ell = T$, with $t_j = j \tau$, $j = 0, 1, \ldots, \ell$ and the time step size $\tau := T/\ell$. We employ the following implicit conforming Galerkin FEM approximation: find $u_h^{j+1} \in V_h$ for $j \in \{0, \cdots, \ell - 1\}$ such that

$$\left\{ \begin{array}{l}
\tau^{-1}(u_h^{j+1} - u_h^j, v_h) + B[u_h^{j+1}, u_h^{j+1}, v_h] + a(u_h^{j+1}, v_h) = 0, \ \forall v_h \in V_h, \\
(u_h^0, v_h) = (u^0, v_h), \ \forall v_h \in V_h.
\end{array} \right. \quad (19)$$

The scheme (19) is well-posed \cite{6, 10}, and satisfies the following stability result \cite{10}.

**Proposition 4.** Let the time step size $\tau > 0$ be sufficiently small. Then problem (19) has a unique solution $u_h^j \in V_h$, and further the following stability estimate holds

$$\|u_h^{j+1}\|_{L^2(D)}^2 + \tau \sum_{k=0}^{j} \|\nabla u_h^{k+1}\|_{L^2(D)}^2 \leq \|u_h^0\|_{L^2(D)}^2, \ \forall j = 0, 1, \cdots, \ell - 1. \quad (20)$$

Now we discuss on the error estimate for the scheme (19), which has a long and rich history (see, e.g., \cite{6, 10–12} for a rather incomplete list). The scheme has a first-order convergence in time, while the convergence order for spatial discretization depends on the regularity of solutions. More precisely, we decompose the error $u(t_j) - u_h^j$ of the fully-discrete scheme (19) into

$$u(t_j) - u_h^j = (u(t_j) - u_h(t_j)) + (u_h(t_j) - u_h^j),$$

where $u_h$ is the solution to the semi-discrete scheme

$$\left\{ \begin{array}{l}
(\partial_t u_h, v_h) + B[u_h, u_h, v_h] + a(u_h, v_h) = 0, \ \forall v_h \in V_h, \\
(u_h^0, v_h) = (u^0, v_h), \ \forall v_h \in V_h.
\end{array} \right. $$

The terms $u(t_j) - u_h(t_j)$ and $u_h(t_j) - u_h^j$ denote the spatial and time discretization errors, respectively. For the spatial error, if $\|u^0\|_{H^2(D)} \leq M$ for some $M > 0$, then \cite[Theorem 4.5]{13} gives

$$\|u(t) - u_h(t)\|_{L^2(D)} \leq C t^{-\frac{1}{2}} h^2, \ \forall t \in (0, T], \quad (21)$$

where the constant $C := C(M, T, D)$ depends only on $M$, $T$ and $D$. Note that the initial data $u^0$ also depends on the stochastic variable $y \in U_b$. Nonetheless, (5) and Assumption 2 guarantee the existence of an $M > 0$ independent of $y \in U_b$ such
that \( \sup_{y \in U_b} \| u^0(y) \|_{H^1(D)} < M \). Thus, the constant \( M \) in (21) can be chosen to be independent of \( y \in U_b \) for the solutions with the stochastic variable \( y \).

For the time error, there are several results depending on the type of temporal discretization [6, 10, 12, 14, 15], under different time regularity assumptions on the solution. Since a detailed discussion of the finite element approximation of the Navier–Stokes equations is not our focus, we will not explicitly specify the regularity assumptions. Instead, we assume the following condition: for any sufficiently small \( h > 0 \),

\[
\mathbb{E} \left[ \| \partial_t u_h(y) \|_{L^2(0,T;V)} + \| \partial_t u_h(y) \|_{L^2(0,T;V')} \right] \leq C,
\]

for some \( C > 0 \) independent of \( y \in U_b \). See, e.g., [15–17] for discussions on similar properties of \( u_h \). Then following the argument of [6, 10], we obtain

\[
\mathbb{E} \left[ \| u_h(t) - u_h^0 \|_{L^2(D)} \right] \leq C \tau, \quad \forall J > 0,
\]

where the constant \( C > 0 \) is independent of \( y \in U_b \).

Summarizing the above discussion and using the linearity of \( \mathcal{G} \) and Hölder’s inequality (for the term related to \( \mathcal{G} \)), we have the following result.

**Theorem 5.** Let \( D \subset \mathbb{R}^2 \) be a convex polygonal domain and \( \mathcal{G} \in (L^2(D)^2)' \), and let Assumption 2 and (22) hold. Then there exists a constant \( C > 0 \) independent of \( y \in U_b \) such that

\[
\mathbb{E}[\mathcal{G}(u(t,J)) - \mathcal{G}(u^0_h)] \leq C(tJ^{-\frac{3}{2}}h^2 + \tau).
\]

### 4 Truncation of the infinite-dimensional problem

The second discretization step reduces the parametric dimension: we truncate the infinite series (10) to a finite-dimensional sum, and obtain a truncated initial data

\[
u^0_s(x, y) = (-\partial_{x^j} \exp Z_x \partial_{x^j} \exp Z_y),
\]

where \( Z_x(\cdot, \cdot) \) is the truncated KL expansion of the random field \( Z(\cdot, \cdot) \), given by

\[
Z_x(x, y) := \sum_{j=1}^s \sqrt{\mu_j} \zeta_j(x)y_j.
\]

Note that \( u^0_s(x, y) \) can be identified as the initial data \( u^0(x, y) \) evaluated at the vector \( y = (y_1, \cdots, y_s, 0, 0, \cdots) \). For any set of ‘active’ coordinates \( \kappa \subset \mathbb{N} \), we denote the vectors \( y \in U_b \) with \( y_j = 0 \) for \( j \notin \kappa \) by \( (y_\kappa; 0) \).

Then consider the following scheme for the truncated problem with the initial data \( u^0_s \): Given \( u_{s,h}^0 \in V_h \), and \( s \in \mathbb{N} \), find \( u_{s+1,h}^0 \in V_h \) such that

\[
t^{-1}(u_{s+1,h}^0 - u_{s,h}^0, v_h) + B(u_{s+1,h}^0, u_{s+1,h}^0, v_h) + a(u_{s+1,h}^0, v_h) = 0, \quad \forall v_h \in V_h, \quad (u_{s,h}^0, v_h) = (u^0_s, v_h), \quad \forall v_h \in V_h,
\]

(25)
where \( u_{0,s}^h \) is the \( L^2(D) \)-projection of \( u_0^0 \) into \( V_h \). The well-posedness of the scheme (25) follows by the argument in Section 3. The next result gives the truncation error.

**Theorem 6.** Let Assumption 2 hold and \( G \in (L^2(D))^\ell \). If the time step size \( \tau > 0 \) is sufficiently small, i.e.,

\[
\tau \| u_h^j \|_{L^\infty(D)} < 1, \quad \forall j > 0 \text{ and } h > 0.
\]

Then for any time level \( j \in \{0, 1, \cdots, \ell\} \), mesh size \( h > 0 \) and parametric dimension \( s \in \mathbb{N} \), there exists \( C > 0 \) independent of \( j, h \) and \( s \) such that

\[
E[|G(u_h^j) - G(u_{s,h}^j)|] \leq C s^{-\frac{3}{2} + \frac{3}{2}}.
\]

**Proof.** First, by Fernique’s theorem in Theorem 17, for any \( s \in \mathbb{N} \), we have

\[
\| \exp(Z) \|_{L^2(\Omega;C(D))} \lesssim 1 \quad \text{and} \quad \| \exp(Z_s) \|_{L^2(\Omega;C(D))} \lesssim 1,
\]

Let \( u_{j,s}^h \) and \( u_{j,s}^{h,\ell} \) be the solution to the scheme (19) and problem (25), respectively, and \( d_{s,h}^j := u_{j,s}^h - u_{j,s}^{h,\ell} \). Then subtracting (19) from (25) and setting \( v_h = d_{s,h}^{j+1} \in V_h \) yield

\[
\tau^{-1}(d_{s,h}^{j+1} - d_{s,h}^j) + (\nabla d_{s,h}^{j+1}, \nabla d_{s,h}^j) = B[u_{j,s}^h, u_{j,s}^{h,\ell}, d_{s,h}^{j+1}] - B[u_{j,s}^h, u_{j,s}^{h,\ell}, d_{s,h}^j].
\]

By the skew symmetry of \( B[\cdot, \cdot, \cdot] \), Hölder’s inequality, Ladyzhenskaya’s inequality in Lemma 15 and Young’s inequality, we deduce

\[
|B[u_{j,s}^h, u_{j,s}^{h,\ell}, d_{s,h}^{j+1}] - B[u_{j,s}^h, u_{j,s}^{h,\ell}, d_{s,h}^j]| \\
= |B[d_{s,h}^{j+1}, u_{j,s}^h, d_{s,h}^j] + B[u_{j,s}^{h,\ell}, d_{s,h}^{j+1}, d_{s,h}^j]| \\
= | - B[d_{s,h}^{j+1}, d_{s,h}^{j+1}, u_{j,s}^{h,\ell}]| \lesssim \| d_{s,h}^{j+1} \|_{L^2(D)} \| \nabla d_{s,h}^{j+1} \|_{L^2(D)} \| u_{j,s}^{h,\ell} \|_{L^4(D)} \\
\lesssim \| d_{s,h}^{j+1} \|_{L^2(D)} \| \nabla d_{s,h}^{j+1} \|_{L^2(D)} \| u_{j,s}^{h,\ell} \|_{L^2(D)} \\
\lesssim \frac{1}{4} \| u_{j,s}^{h,\ell} \|_{L^2(D)}^2 + \frac{1}{4} \| \nabla d_{s,h}^{j+1} \|_{L^2(D)}^2.
\]

Using the identity \( \tau^{-1}(d_{s,h}^{j+1} - d_{s,h}^j, d_{s,h}^{j+1}) = (2\tau)^{-1}(\| d_{s,h}^{j+1} \|^2 - \| d_{s,h}^j \|^2 + \| d_{s,h}^{j+1} - d_{s,h}^j \|^2) \), and summing up the previous results from \( j = 0 \) to \( j = k - 1 \) for \( k \geq 1 \) yields

\[
\| d_{s,h}^k \|_{L^2(D)}^2 + \frac{k-1}{2} \sum_{j=0}^{k-1} \| \nabla d_{s,h}^{j+1} \|_{L^2(D)}^2 \lesssim \| d_{s,h}^0 \|_{L^2(D)}^2 + \frac{k-1}{2} \sum_{j=0}^{k-1} \| u_{j,s}^{h,\ell} \|_{L^4(D)}^2 \| d_{s,h}^{j+1} \|_{L^2(D)}^2.
\]

Then (26) and the discrete Gronwall’s inequality in Lemma 16 imply

\[
\| d_{s,h}^k \|_{L^2(D)}^2 \lesssim \| d_{s,h}^0 \|_{L^2(D)}^2 \exp \left( \frac{k-1}{2} \sum_{j=0}^{k-1} \frac{\| u_{j,s}^{h,\ell} \|_{L^4(D)}^2}{1 - \tau \| u_{j,s}^{h,\ell} \|_{L^4(D)}^2} \right)
\]
\[ \lesssim \|d_{s,h}^0\|^2_{L^2(D)} \exp \left( C\tau \sum_{j=0}^{k-1} \|u_h^{j+1}\|^4_{L^4(D)} \right). \]

Note that the exponential term on the right-hand side is uniformly bounded in $k \geq 1$. Indeed, Proposition 4 and Ladyzhenskaya’s inequality (cf. Lemma 15 in the appendix) yield the following $L^4(D)$-estimate on $u_h^j$

\[ \tau \sum_{k=0}^{j-1} \|u_h^{k+1}\|^4_{L^4(D)} \leq 2\|u_h^0\|^4_{L^4(D)}. \tag{29} \]

Further, by taking $v_h = u_h^0 - u_{s,h}^0$ in the definition of $L^2$-projection, i.e., $(u^0 - u_s^0, v_h) = (u_h^0 - u_{s,h}^0, v_h)$, and Hölder’s inequality, we deduce

\[ \|u_h^0 - u_{s,h}^0\|_{L^2(D)} \leq \|u^0 - u_s^0\|_{L^2(D)} \lesssim \|u^0 - u_s^0\|_{C(D)}, \]

since the domain $D$ is bounded. To estimate $\|u^0 - u_s^0\|_{C(D)}$, we derive from the definitions of $u^0$ and $u_s^0$ that

\[
\begin{align*}
E \left[ \|u^0 - u_s^0\|_{C(D)} \right] &= E \left[ \|(-\partial_{x^2} Z \exp(Z) + \partial_{x^2} Z_s \exp(Z_s) - \partial_{x^2} Z_s \exp(Z_s))\|_{C(D)} \right] \\
& \lesssim \sum_{i=1}^2 E \left[ \|\partial_{x^2} Z \exp(Z) - \partial_{x^2} Z_s \exp(Z_s)\|_{C(D)} \right].
\end{align*}
\]

Then the triangle inequality, Hölder’s inequality, Assumption 2 and Sobolev embedding yield

\[
\begin{align*}
& E \left[ \|\partial_{x^2} Z \exp(Z) - \partial_{x^2} Z_s \exp(Z_s)\|_{C(D)} \right] \\
& \lesssim E \left[ \|\partial_{x^2} Z \exp(Z) - \partial_{x^2} Z_s \exp(Z_s)\|_{C(D)} \right] + E \left[ \|\partial_{x^2} Z_s \exp(Z_s) - \partial_{x^2} Z_s \exp(Z_s)\|_{C(D)} \right] \\
& \lesssim E \left[ \|\partial_{x^2} Z\|_{C(D)} \right] \|\exp(Z) - \exp(Z_s)\|_{C(D)} + E \left[ \|\exp(Z_s)\|_{C(D)} \|\partial_{x^2} Z - \partial_{x^2} Z_s\|_{C(D)} \right] \\
& \lesssim E \left[ \|\exp(Z) - \exp(Z_s)\|_{C(D)} \right] + E \left[ \|\exp(Z_s)\|_{C(D)}^2 \right]^{1/2} \times E \left[ \|\partial_{x^2} Z - \partial_{x^2} Z_s\|_{C(D)}^2 \right]^{1/2} \\
& =: I + II \times III.
\end{align*}
\]

Note that under Assumption 2, for sufficiently large $s \in \mathbb{N}$, there holds \[18\]

\[ \|Z - Z_s\|_{L^\infty(\Omega;C(D))} \lesssim s^{-\frac{1}{2}+1}. \tag{30} \]

Thus, for the term $I$, it follows from the inequality $|e^x - e^y| \leq |x - y|(e^x + e^y)$ for any $x, y \in \mathbb{R}$, Hölder’s inequality, and \[27\] that

\[
I \lesssim E \left[ \|Z - Z_s\|_{C(D)} \right] \|\exp(Z) + \exp(Z_s)\|_{C(D)}
\]
\[ \|Z - Z_s\|_{L^2(\Omega)} \|\exp(Z) + \exp(Z_s)\|_{L^2(\Omega)} \leq \|Z - Z_s\|_{L^2(\Omega)} \|\exp(Z)\|_{L^2(\Omega)} + \|\exp(Z_s)\|_{L^2(\Omega)} \leq s^{-\frac{1}{2}+1}. \]

Meanwhile, (27) directly implies \( II \leq 1 \). Since \( \{y_j(\omega)\}_{j \in \mathbb{N}} \) is orthonormal in \( L^2(\Omega) \), using the estimates (12) and (13) leads to

\[ III = \left\| \sum_{j \geq s} \sqrt{n_j} \partial_{x_j} \xi_j y_j \right\|_{L^2(\Omega)} \leq \left\| \sum_{j \geq s} \sqrt{n_j} \partial_{x_j} \xi_j \right\|_{L^2(\Omega)} \leq \left( \sum_{j > s} \mu_j \|\partial_{x_j} \xi_j\|_{L^2(\Omega)}^2 \right)^{1/2} \leq \left( \int_s^\infty t^{-k+2} \, dt \right)^{1/2} \lesssim s^{-\frac{1}{2}+\frac{1}{2}}, \]

upon noting \( k > 2 \) in Assumption 2. Finally, we derive

\[ \mathbb{E}[\|G(u^I_s) - G(u^J_s)\|] = \mathbb{E}[\|G(u^I_s - u^J_s)\|] \lesssim \mathbb{E}[\|u^I_s - u^J_s\|_{L^2(\Omega)}] \lesssim \mathbb{E}[\|u^0 - u^0\|_{L^2(\Omega)}] \lesssim s^{-\frac{1}{2}+\frac{1}{2}}. \]

Combining the preceding estimates proves the desired assertion. \( \square \)

**Remark 1.** The estimate (29) implies \( \tau \|u^I_s\|^4_{L^2(\Omega)} \leq 2 \|u^0\|^4_{L^2(\Omega)} \) for all \( j \geq 0 \) and \( h > 0 \). Below we shall assume the smallness of initial data \( \|u^0\| \leq \varepsilon \approx \tau^{1/2} \). Thus, for sufficiently small \( \tau > 0 \), the condition (26) holds independently of \( j \geq 1 \) and \( h > 0 \).

## 5 Quasi-Monte Carlo integration

Now we use QMC to approximate the linear functional \( G \in (L^2(\Omega))^\ell \), i.e., \( \mathbb{E}[G(u^J_s)] \).

More precisely, given parametric dimension \( s \in \mathbb{N} \), time level \( J \in \{1, \cdots, \ell\} \) and mesh size \( h > 0 \), we approximate \( \mathbb{E}[G(u^J_s)] \) by the following integral

\[ I_s(F^J_s) := \int_{\mathbb{R}^s} F^J_s(y) \prod_{j=1}^s \phi(y_j) \, dy, \quad \text{with} \quad F^J_s(y) := G(u^J_s(y)). \quad (31) \]

Here, \( \phi(y) := \exp(-y^2/2)/\sqrt{2\pi} \) and \( \Phi(y) = \int_{-\infty}^y \exp(-t^2/2)/\sqrt{2\pi} \, dt \) is the standard Gaussian PDF and CDF, respectively. To apply QMC methods, we transform the integral (31) over the unbounded domain \( \mathbb{R}^s \) to a hyper-cube \( [0,1]^s \) by introducing new variables \( y = \Phi^{-1}(v) \), where \( \Phi^{-1}(v) \) is the inverse CDF for \( v \in [0,1]^s \). Then changing variables yields

\[ \mathbb{E}[G(u^J_s)] = \mathbb{E}[F^J_s] = \int_{(0,1)^s} F^J_s(\Phi^{-1}(v)) \, dv. \]
We approximate the integral on $(0, 1)^s$ by a randomly-shifted lattice rule (RSLR):

$$Q_{s,N}(F^J_{s,h}; \Delta) := \frac{1}{N} \sum_{i=1}^{N} F^J_{s,h} \left( \Phi^{-1} \left( \frac{i z}{N} + \Delta \right) \right), \quad (32)$$

where $z \in \mathbb{N}^s$ is a deterministic generating vector and $\Delta$ is a uniformly distributed random shift over $[0, 1]^s$. We shall establish an $O(N^{-1})$ bound on

$$\text{RMSE}_{\text{qmc}}(N) := \left( \mathbb{E}_{\Delta} \left[ \left( \mathbb{E}\left[ G(u^J_{s,h}) \right] - Q_{s,N}(F^J_{s,h}; \Delta) \right)^2 \right] \right)^{1/2},$$

where $\mathbb{E}_{\Delta}$ denotes taking expectation in the random shift $\Delta \in [0, 1]^s$, with a constant independent of $s \in \mathbb{N}$, $J \in \mathbb{N}$ and $h > 0$.

### 5.1 Solution regularity in the stochastic variables

First we bound mixed first derivatives of $u^J_{s,h}(y)$ with respect to the parametric variable $y \in U_b$. This represents the main technical challenge in the QMC analysis. Below $u = (u_j)_{j \in \mathbb{N}}$ denotes the standard multi-index of non-negative integers with $|u| = \sum_{j \geq 1} u_j < \infty$, and $\partial^u u$ denotes the mixed derivative of $u$ with respect to all variables in the multi-index $u$. We focus on the mixed first derivative $\partial^u$, i.e., $u_j \in \{0, 1\}$ for all $j \in \mathbb{N}$. By Assumption 3, there exists $N_0 \in \mathbb{N}$ sufficiently large such that $j > N_0$ implies $b_j \leq \frac{1}{2}$. Then we define a positive sequence $\{C_j\}_{j=1}^{\infty}$ by

$$C_j := \begin{cases} \max\{2b_j, 1\} & \text{if } j \in \{1, \cdots, N_0\}; \\ 1 & \text{if } j > N_0. \end{cases} \quad (33)$$

Then the constant $C^* > 0$, defined by

$$C^* := \prod_{j \geq 1} C_j = \prod_{j=1}^{N_0} \max\{2b_j, 1\}, \quad (34)$$

is finite, i.e., $C^* < \infty$.

Now we estimate mixed first derivatives of the discrete truncated initial data $u_{s,h}^0$.

**Lemma 7.** Let $\partial^u$ be a mixed first derivative with respect to $y$ and let Assumption 3 hold. Then the following estimate holds

$$\|\partial^u u^0_s\|_{L^2(D)} \leq 2^{-|u|}(C^* + 2\sqrt{2})|u| \| \exp Z_s(\cdot, y) \|_{H^1(D)}. \quad (35)$$

**Proof.** By the definition of $L^2(D)$-projection $u^0_{s,h}(y)$, for each $y \in U_b$, we have

$$(u^0_{s,h}(y), v_h) = (u^0_s(y), v_h), \quad \forall v_h \in V_h.$$
Taking $\partial^u$ on both sides and then setting $v_h = \partial^u u^0_{s,h} \in V_h$ yield that for each $y \in U_b$,

$$\|\partial^u u^0_{s,h}(y)\|_{L^2(D)}^2 = (\partial^u u^0_{s,h}(y), \partial^u u^0_{s,h}(y)) \leq \|\partial^u u^0_{s,h}(y)\|_{L^2(D)} \|\partial^u u^0_{s,h}(y)\|_{L^2(D)},$$

Hence, we have

$$\|\partial^u u^0_{s,h}(y)\|_{L^2(D)} \leq \|\partial^u u^0_{s,h}(y)\|_{L^2(D)}. \quad (36)$$

With the notation $j \in u$ when $u_j = 1$, by the product rule,

$$\|\partial^u u^0_s\|_{L^2(D)} = \|\partial^u \partial_x \exp Z_s\|_{L^2(D)} = \|\partial_x \left[ \left( \prod_{j \in u} \sqrt{\mu_j} \xi_j \right) \exp Z_s \right]\|_{L^2(D)}$$

$$\leq \left\| \left( \prod_{j \in u} \sqrt{\mu_j} \xi_j \right) \partial_x \exp Z_s \right\|_{L^2(D)} + \left\| \prod_{j \in u, j \neq i} \sqrt{\mu_j} \partial_x \xi_i \left( \prod_{j \in u, j \neq i} \sqrt{\mu_j} \xi_j \right) \exp Z_s \right\|_{L^2(D)} =: I + II.$$

By (33) and (34), the following inequality holds

$$\prod_{j \in u} b_j = \prod_{j \in u, j > N_0} b_j \times \prod_{j \in u, j \leq N_0} b_j \leq \prod_{j \in u, j > N_0} \frac{1}{2} \times \prod_{j \in u, j \leq N_0} \frac{C_j}{2} \leq \frac{C^*}{2|u|}.$$

Then we can bound the first term $I$ by

$$I \leq \left( \prod_{j \in u} b_j \right) \|\partial_x \exp Z_s\|_{L^2(D)} \leq \frac{C^*}{2|u|} \|\partial_x \exp Z_s\|_{L^2(D)}.$$

For the term $II$, we discuss the cases $|u| \geq 2$ and $|u| = 1$ separately. When $|u| \geq 2$, the estimates (12) and (13) imply

$$II \leq \|\exp Z_s\|_{L^2(D)} \sum_{i \in u} \sqrt{\mu_i} \|\partial_x \xi_i\|_{L^2(D)} \left( \prod_{j \in u, j \neq i} b_j \right) \leq \|\exp Z_s\|_{L^2(D)} \sum_{i \in u} i^{-\frac{3}{2} + 1} \left( \prod_{j \in u, j \neq i} j^{-\frac{3}{2} + \frac{3}{2}} \right).$$

Plugging the following identity

$$\sum_{i \in u} i^{-\frac{3}{2} + 1} \left( \prod_{j \in u, j \neq i} j^{-\frac{3}{2} + \frac{1}{2}} \right) = \sum_{i \in u} i^{-\frac{3}{2} + 1} \left( \prod_{j \in u, j \neq i} j^{-\frac{3}{2} + \frac{3}{2}} \right)$$

$$= \sum_{i \in u} \left( \prod_{j \in u} j^{-\frac{3}{2} + 1} \right) \left( \prod_{j \in u, j \neq i} j^{-\frac{1}{2}} \right)$$

into the last inequality leads to

$$II \leq \|\exp Z_s\|_{L^2(D)} \sum_{i \in u} \left( \prod_{j \in u} j^{-\frac{3}{2} + 1} \right) \left( \prod_{j \in u, j \neq i} j^{-\frac{1}{2}} \right)$$
$$= \| \exp Z_s \|_{L^2(D)} \left( \prod_{j \in n} j^{-\frac{k-2}{2}} \right) \sum_{i \in N} \left( \prod_{j \in n, j \neq i} j^{-\frac{1}{2}} \right).$$

Upon noting $k > 3$, we deduce

$$\Pi \leq \| \exp Z_s \|_{L^2(D)} \frac{1}{(2^{\frac{k-2}{2}})^{|u|-1}} \sum_{i \in n} \left( \prod_{j \in n, j \neq i} j^{-\frac{1}{2}} \right) \leq \| \exp Z_s \|_{L^2(D)} \frac{2\sqrt{2}|u|}{2^{|u|}}.$$
$$+ \sum_{m \geq u} \binom{u}{m} B[\partial^{u-m} u_{s,h}^{j+1}, \partial^m u_{s,h}^{j+1}, v_h] = 0, \quad \forall v_h \in V_h,$$

where $m \leq u$ denotes $m_j \leq u_j$ for all $j \geq 1$, and $u - m$ is a multi-index $(u_j - m_j)_{j \geq 1}$ and $\binom{u}{m} := \prod_{j \geq 1} \binom{u_j}{m_j}$. Upon splitting the summation with $m \neq u$ (i.e., $\neq u$), we obtain

$$\left( \nabla \partial^u u_{s,h}^{j+1}, \nabla v_h \right) + B[u_{s,h}^{j+1}, \partial^u u_{s,h}^{j+1}, v_h] + \tau^{-1}(\partial^u u_{s,h}^{j+1}, v_h)$$

$$- \tau^{-1}(\partial^u u_{s,h}^{j+1}, v_h) = - \sum_{m \geq u} \binom{u}{m} B[\partial^{u-m} u_{s,h}^{j+1}, \partial^m u_{s,h}^{j+1}, v_h], \quad \forall v_h \in V_h.$$

Upon taking $v_h := 2\tau \partial^u u_{s,h}^{j+1}$ in the identity, we obtain

$$2\tau \| \nabla \partial^u u_{s,h}^{j+1} \|_{L^2(D)} + \| \partial^u u_{s,h}^{j+1} \|_{L^2(D)} - \| \partial^u u_{s,h}^{j+1} - \partial^u u_{s,h}^{j+1} \|_{L^2(D)}^2$$

$$= - 2\tau \sum_{m \geq u} \binom{u}{m} B[\partial^{u-m} u_{s,h}^{j+1}, \partial^m u_{s,h}^{j+1}, \partial^u u_{s,h}^{j+1}]. \quad (39)$$

The skew symmetry of the trilinear form $B[\cdot, \cdot, \cdot]$ implies

$$B[\partial^{u-m} u_{s,h}^{j+1}, \partial^m u_{s,h}^{j+1}, \partial^u u_{s,h}^{j+1}] \leq \frac{1}{2} \| \partial^{u-m} u_{s,h}^{j+1} \|_{L^2(D)} \| \nabla \partial^m u_{s,h}^{j+1} \|_{L^2(D)} + \frac{1}{2} \| \partial^u u_{s,h}^{j+1} \|_{L^2(D)} \| \nabla \partial^m u_{s,h}^{j+1} \|_{L^2(D)} \| \partial^u u_{s,h}^{j+1} \|_{L^2(D)}.$$

By bounding the terms $\| \partial^{u-m} u_{s,h}^{j+1} \|_{L^2(D)}$, $\| \partial^m u_{s,h}^{j+1} \|_{L^2(D)}$, and $\| \partial^u u_{s,h}^{j+1} \|_{L^2(D)}$ using Ladyzhenskaya’s inequality in Lemma 15 and then applying Poincaré’s inequality (with Poincaré constant $C_p$), we deduce

$$\left| - \sum_{m \geq u} \binom{u}{m} B[\partial^{u-m} u_{s,h}^{j+1}, \partial^m u_{s,h}^{j+1}, \partial^u u_{s,h}^{j+1}] \right|$$

$$\leq \sqrt{2} C_p \sum_{m \geq u} \binom{u}{m} \| \nabla \partial^{u-m} u_{s,h}^{j+1} \|_{L^2(D)} \| \nabla \partial^m u_{s,h}^{j+1} \|_{L^2(D)} \| \partial^u u_{s,h}^{j+1} \|_{L^2(D)}.$$

Together with (39), we arrive at

$$2\tau \| \nabla \partial^u u_{s,h}^{j+1} \|_{L^2(D)}^2 + \| \partial^u u_{s,h}^{j+1} \|_{L^2(D)}^2 - \| \partial^u u_{s,h}^{j+1} - \partial^u u_{s,h}^{j+1} \|_{L^2(D)}^2$$

$$\leq 2\sqrt{2} C_p \tau \sum_{m \geq u} \binom{u}{m} \| \nabla \partial^{u-m} u_{s,h}^{j+1} \|_{L^2(D)} \| \nabla \partial^m u_{s,h}^{j+1} \|_{L^2(D)} \| \partial^u u_{s,h}^{j+1} \|_{L^2(D)}.$$

For fixed $J = 2, \cdots, \ell$, let $S_u^{J} := (\Delta t \sum_{j=0}^{J-1} \| \nabla \partial^u u_{s,h}^{j+1} \|_{L^2(D)}^2)^{1/2}$. Summing up from $j = 0$ to $j = J - 1$, using Cauchy–Schwarz inequality and (36) yield

$$\| \partial^u u_{s,h}^{J} \|_{L^2(D)}^2 + 2 S_u^{J} \leq \| \partial^u u_{s,h}^{0} \|_{L^2(D)}^2.$$

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Now we choose $\varepsilon := 2$ which implies $S = 2$.

To estimate $S^J_u$ when $|u| = 0$, by taking $v_h = 2\tau u_{s,h}^{j+1}$ in (25) and Young’s inequality,

$$2\|u_{s,h}^{j+1}\|^2_{L^2(D)} + 2\tau \|\nabla u_{s,h}^{j+1}\|^2_{L^2(D)} = (u_{s,h}^{j+1}, u_{s,h}^{j+1}) \leq \|u_{s,h}^{j+1}\|^2_{L^2(D)} + \|u_{s,h}^{j+1}\|^2_{L^2(D)},$$

which implies $\|u_{s,h}^{j+1}\|^2_{L^2(D)} + 2\tau \|\nabla u_{s,h}^{j+1}\|^2_{L^2(D)} \leq \|u_{s,h}^{j+1}\|^2_{L^2(D)}$. Summing the above inequality from $j = 0$ to $j = J - 1$ yields

$$2(S^0_u)^2 \leq \|u_{s,h}^{J}\|^2_{L^2(D)} + 2\tau \sum_{j=0}^{J-1} \|\nabla u_{s,h}^{j+1}\|^2_{L^2(D)} \leq \|u_{s,h}^{0}\|^2_{L^2(D)} \leq \exp Z_s\|H^1(D).$$

Now we choose $\varepsilon := \frac{1}{4A(C^2 + 2\sqrt{2})}$, which is proportional to $\tau^{1/2}$, and assume the smallness condition (37). Then we prove the claim

$$S^J_u \leq |u|^{2M} \|\partial^u u^0\|^2_{L^2(D)}, \quad \forall J \in \mathbb{N}$$

by mathematical induction on $|u|$. For $|u| = 1$, from (40) and (41), we have

$$2(S^J_u)^2 \leq AS^0_u(S^J_u)^2 + \|\partial^u u^0\|^2_{L^2(D)} \leq A\|Z_s\|_{H^1(D)}(S^J_u)^2 + \|\partial^u u^0\|^2_{L^2(D)}.$$

This, the smallness assumption (37) and the choice of $\varepsilon$ imply the inequality (42) when $|u| = 1$. Now suppose that (42) holds for all $u$ with $1 \leq |u| \leq n - 1, n \geq 2$. For any given multi-index $u$ with $|u| = n$, it follows from (40) and (41) that

$$2(S^J_u)^2 \leq A\sum_{m \geq u, m \neq 0} S^J_{u-m} S^J_{m} S^J_{u} + \frac{A}{2}|\exp Z_s\|_{H^1(D)}(S^J_u)^2 + \|\partial^u u^0\|^2_{L^2(D)}.$$
By the induction hypothesis, (35) and the smallness assumption (37), we have

\[
\frac{(S_u^{j})^2}{2} \leq A \sum_{i=1}^{[n]-1} \sum_{|m|=i} \|\partial^m u_0^0\|_{L^2(D)}^2 |u - m!2^{[m]}| m!2^{m} |S_u^{j}| + \|\partial^m u_0^0\|_{L^2(D)}^2
\]

\[
\leq A \|\partial^m u_0^0\|_{L^2(D)}^2 (|u| - 1)2^{|u|} \sum_{i=1}^{[n]-1} \left( \begin{array}{c} |u| \\ i \end{array} \right) S_u^{j} + \|\partial^m u_0^0\|_{L^2(D)}^2
\]

\[
\leq A \|\partial^m u_0^0\|_{L^2(D)}^2 (|u| - 1)2^{|u|} (2^{|u|} - 2) S_u^{j} + \|\partial^m u_0^0\|_{L^2(D)}^2,
\]

\[
\leq A(C^* + 2\sqrt{2}) \|\exp Z_{u} \|_{L^2(D)} \|\partial^m u_0^0\|_{L^2(D)} \|u| |2^{|u|} S_u^{j} + \|\partial^m u_0^0\|_{L^2(D)}^2,
\]

\[
\leq \frac{1}{2} \|\partial^m u_0^0\|_{L^2(D)} \|u| |2^{|u|} S_u^{j} + \|\partial^m u_0^0\|_{L^2(D)}^2,
\]

using the inequality \(a!b! \leq (a+b-1)!\) for any \(a, b \in \mathbb{N}\). Solving the quadratic inequality for \(S_u^{j}\) yields the claim (42):

\[
S_u^{j} \leq \frac{1}{2} \|\partial^m u_0^0\|_{L^2(D)} \|u| |2^{|u|} + \sqrt{2} \|\partial^m u_0^0\|_{L^2(D)} \leq |u| |2^{|u|} \|\partial^m u_0^0\|_{L^2(D)}.
\]

Last, substituting (42) into (40) and repeating the above argument yield

\[
\|\partial^m u_0^0\|_{L^2(D)} \leq \frac{1}{2} \|\partial^m u_0^0\|_{L^2(D)} (|u|)! |2^{|u|} \|\partial^m u_0^0\|_{L^2(D)} + \|\partial^m u_0^0\|_{L^2(D)}^2,
\]

This, together with (35), implies

\[
\|\partial^m u_0^0\|_{L^2(D)} \leq 2|u| |2^{|u|} \|\partial^m u_0^0\|_{L^2(D)} \leq (2\sqrt{2} + 2C^*) |u| |2^{|u|} \|\exp Z_{u} \|_{H^1(D)}.
\]

This completes the proof of the theorem. \(\square\)

5.2 A function space setting in \(\mathbb{R}^s\)

The "standard" function spaces in the QMC analysis are weighted Sobolev spaces on (0, 1)^s, which consists of functions with square-integrable mixed first derivatives. If the integrand lies in a suitable weighted Sobolev space, randomly-shifted lattice rules (RSLRs) can be constructed so as to (nearly) achieve the convergence rate \(O(n^{-1})\); see [21–25] and recent surveys [26, 27]. Since the integral in (31) is defined over \(\mathbb{R}^s\), we have first transformed the domain to (0, 1)^s and obtain \(F_0^j(\Phi_{i-1}(\cdot))\). However, the resulting integrand may be unbounded near the boundary \(\partial(0, 1)^s\), and thus the standard QMC theory is not directly applicable. The function space setting for the integral of the type (31) has been studied in [28–33], and the optimal convergence rate has been obtained using RSLRs. The corresponding weighted Sobolev norm is defined by [32, 33]

\[
\|F\|_{\mathcal{W}_{\gamma}} := \sum_{u \subset [s]} \frac{1}{\gamma_u} \int_{\mathbb{R}^{|u|}} \int_{\mathbb{R}^{|u|}} \partial^m F(y_u; y_{[s]\setminus u}) \prod_{j \in [s]\setminus u} \phi(y_j) dy_{[s]\setminus u} \prod_{j \in u} \psi^2(y_j) dy_u,
\]

(43)
where \([s] = \{1, 2, \cdots, s\}\), \(\partial^u F\) denotes the mixed first derivative with respect to each “active” variables \(y_j\) for \(j \in u\), and \(y_{[u]\setminus u}\) is the “inactive” variable \(y_j, j \notin u\). The norm (31) is called “unanchored” since the inactive variables are integrated out as opposed to being “anchored” at a certain fixed value, e.g., 0.

For each \(j \geq 1\), the continuous weight function \(\psi_j : \mathbb{R} \to \mathbb{R}_+\) in (43) should be properly chosen to handle the singularities for the active variables. The analysis in [33] indicates that \(\psi_j^2(y)\) should decay slower than the standard Gaussian density in (31) as \(|y| \to \infty\): for some \(a_j > 0\), such that

\[
\psi_j^2(y) = \exp(-2a_j |y|).
\]

(44)

Throughout, we assume that for some constants \(0 < a_{\min} < a_{\max} < \infty\),

\[
a_{\min} < a_j \leq a_{\max}, \quad j \in \mathbb{N}.
\]

(45)

For each index \(u \subset \mathbb{N}\) with finite cardinality \(|u| < \infty\), we associate a weight parameter vector \(\gamma_u > 0\) to indicate the relative importance of the variables. We write \(\gamma = (\gamma_u)_{u \subset \mathbb{N}}\) and let \(\gamma_\emptyset := 1\). In [32], only “products weights” were considered, i.e., there exists a sequence \(\gamma_1 \geq \gamma_2 \geq \cdots > 0\), where each \(\gamma_j\) is associated with an integral variable \(y_j\) and let \(\gamma_u := \prod_{j \in u} \gamma_j\). See also [33] for further generalizations. The choice of the weight parameters \(\gamma_u\) is important to guarantee that the constant in the QMC error bound does not grow exponentially as \(s \to \infty\). In this work, we employ the so-called “product and order dependent weights” (“POD” weights) introduced in [34]. Specifically, we consider two different sequences \(\Gamma_0 = \Gamma_1 = 1, \Gamma_2, \ldots, \Gamma_s\) and \(\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_s > 0\) such that \(\gamma_u := \Gamma_{|u|} \prod_{j \in u} \gamma_j\).

5.3 Error bound for randomly-shifted lattice rules

To bound the error of the QMC integration, we define the worst-case error \(e_{\text{wor}}(z, \Delta)\) of the shifted lattice rule (32): for a generating vector \(z\) and a random shift \(\Delta\), \(e_{\text{wor}}(z, \Delta) := \sup_{|F| \leq 1} |I_s(F) - Q_{s,N}(F; \Delta)|\), where \(I_s\) is the integral defined in (31). By the linearity of integration, we have

\[
|I_s(F^{J^*_s}_{sh}) - Q_{s,N}(F^{J^*_s}_{sh}; \Delta)| \leq e_{\text{wor}}(z, \Delta) \|F^{J^*_s}_{sh}\|_{W_s}.
\]

In this work, we consider the root-mean-square error (RMSE) for QMC:

\[
\text{RMSE}_{\text{qmc}}(N) \leq e_{\text{sh}}(z) \|F^{J^*_s}_{sh}\|_{W_s},
\]

(46)

with \(e_{\text{sh}}(z) := \left(\int_{[0,1]^s} (e_{\text{sh}}(z, \Delta))^2 \, d\Delta\right)^{1/2}\) (often known as shift-averaged worst case error). By (46), we can decouple the dependence on \(z\) from that on the integrand \(F^{J^*_s}_{sh}\).

A generating vector \(z = (z_1, z_2, z_3, \cdots)\) can be constructed by a component-by-component algorithm which determines \(z_1, z_2, z_3, \cdots\) sequentially, using \(e_{\text{sh}}(z)\) as the search criterion: given that \(z_1, \cdots, z_i\) are already determined, \(z_{i+1}\) is chosen from the set \(\{1 \leq z \leq N - 1 : \gcd(z, N) = 1\}\) to minimize \(e_{\text{sh}}(z_1, \cdots, z_i, z_{i+1})\). See [33] for the
precise formula for $e_{s,N}^b(z)$ for general weight functions $\psi_j$ and weight parameters $\gamma_u$:

$$(e_{s,N}^b(z))^2 = \sum_{\emptyset \neq u \subseteq \{1, ..., N\}} \frac{\gamma_u}{N} \sum_{i=1}^N \prod_{k \in u} \theta_k \left(\left\{\frac{iz_k}{N}\right\}\right),$$

with

$$\theta_k(f) = \int_{-\infty}^{\infty} \frac{\Phi(t) - f}{\psi^2_k(t)} \, dt + \int_{-\infty}^{\infty} \frac{\Phi(t) - 1 + f}{\psi^2_k(t)} \, dt - \int_{-\infty}^{\infty} \frac{\Phi^2(t)}{\psi^2_k(t)} \, dt.$$

See also [33] for the following choices of $\phi$ and $\psi_k$ with a nearly $O(N^{-1})$ convergence rate: the standard Gaussian CDF and weight functions in (44). Below we use a result from [35]. Note here that $\varphi(p) = p - 1$ for $p$ prime, and it is known that $\frac{1}{\varphi(N)} < \frac{9}{N}$ for any $N \leq 10^{30}$ [3]. Hence, in practice, we can replace $\varphi(N)$ by $\frac{C}{N}$ for some $C > 0$.

**Theorem 9.** For given $h > 0$, $s, J, N \in \mathbb{N}$, weight parameters $\gamma = (\gamma_u)_{u \subseteq \mathbb{N}}$, Gaussian density function $\phi$ and weight function $\psi_j$ defined in (44), an RSLR with $N$ points can be constructed by a component-by-component algorithm satisfying for any $\lambda \in (1/2, 1]$,

$$\text{RMSE}_{\text{qmc}}(N) \leq \left(\sum_{\emptyset \neq u \subseteq \{1, ..., N\}} \gamma_u \prod_{i \in u} \phi_i(\lambda)\right)^{\frac{1}{2N}} |\varphi(N)|^{-\frac{1}{2N}} \|F^J_{s,h}\|_{W_s},$$

with

$$\phi_i(\lambda) := 2 \left(\frac{\sqrt{2\pi} \exp(a_i^2/\eta)}{\pi^{\frac{3}{2}} \exp(1 - \eta \eta)}\right) ^\lambda \zeta\left(\lambda + \frac{1}{2}\right) \quad \text{and} \quad \eta := \frac{2\lambda - 1}{4\lambda}, \quad (47)$$

where $\varphi(n) := \{1 \leq z \leq n - 1 : \gcd(z, n) = 1\}$ is the Euler totient function and $\zeta(x) := \sum_{k=1}^{\infty} k^{-x}$ denotes the Riemann zeta function.

### 5.4 Estimate for the weighted Sobolev norm

The next result shows that for each $s \in \mathbb{N}$ and choice of $\gamma_u$, we have $\|F^J_{s,h}\|_{W_s} < \infty$ for all $J \in \mathbb{N}$ and $h > 0$. Thus, together with Theorem 9, we obtain an estimate for the RMSE$_{\text{qmc}}$ with a nearly $O(N^{-1})$ convergence rate. However, the bound may depend on the parametric dimension $s \in \mathbb{N}$. In Section 5.5, we prove that a careful choice of $\gamma_u$ can remove the dependency on $s \in \mathbb{N}$.

**Theorem 10.** Let the weight functions $\psi_j$ be defined in (44) and $F^J_{s,h}$ the integrand in (31) for any $J = 1, \cdots, \ell$ and $h > 0$. Then $F^J_{s,h} \in W_s$, and with constants $a_i$ and $b_i$ defined in (44) and (14), its $W_s$ norm is bounded by

$$\|F^J_{s,h}\|_{W_s}^2 \leq (2\sqrt{2} + 2C^*)^2 \|\mathcal{U}\|_{L^2(D)}^2 \sum_{u \subseteq \{1, ..., s\}} \frac{(|u|^2)^2 |2|}{\gamma_u} \prod_{i \in u} \frac{b_i^2}{a_i}. \quad (48)$$

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Proof. By Theorem 8 and the linearity of $G$, we obtain for each $y \in \mathbb{R}^s$,

$$|\partial^u F_{s,h}^J(y)| \leq \|G\|_{(L^2(D))^r}^2 \|\partial^u u_{s,h}^J(y)\|_{2} \leq \tilde{C}|u|2^{|u|} \left( \prod_{i \in u} b_i \right) \|Z_s(y)\|_{H^1(D)},$$

with $\tilde{C} := (2\sqrt{2} + 2C^*)\|G\|_{(L^2(D))^r}^2$. Further, the smallness of the truncated log-normal random field (38) implies that $\|\exp Z_s(y)\|_{H^1(D)} \leq 1$ for all $s \in \mathbb{N}$ and $y \in \mathbb{R}^s$. Then the definition of the weighted Sobolev norm (43) implies

$$\|F_{s,h}^J\|_{W_s^2}^2 \leq \tilde{C}^2 \sum_{u \in [s]} \left( \frac{|u|!^22^{|u|}}{\gamma_u} \prod_{j \in u} b_j \right)^2 \int_{\mathbb{R}^{|u|}} \left( \int_{\mathbb{R}^{<|u|}} \prod_{j \in [s] \setminus u} \phi(y_j) dy_j \psi_s(y) \right)^2 \prod_{j \in u} \psi_j^2(y) dy_u$$

$$\leq \tilde{C}^2 \sum_{u \in [s]} \left( \frac{|u|!^22^{|u|}}{\gamma_u} \prod_{j \in u} b_j \right)^2 \prod_{j \in u} a_j,$$

since $\int_{\mathbb{R}} \phi(y) dy = 1$ and $\int_{\mathbb{R}} \psi_j^2(y) dy = \frac{1}{a_j}$ for all $j \in \mathbb{N}$.

Theorems 9 and 10 together give the following RMSE estimate.

**Theorem 11.** Let $F_{s,h}^J$ be the integrand defined in (31) and let $\psi_j$ be a weight function defined in (44). For given $s, J, N \in \mathbb{N}$ with $N \leq 10^30$, $h > 0$, weights $\gamma = (\gamma_u)_{u \in [s]}$ and standard Gaussian density function $\phi$, we can construct an RSLR with $N$ points in $s$ dimensions by a component-by-component algorithm such that for any $\lambda \in (1/2, 1]$,

$$\text{RMSE}_{\text{qmc}}(N) \leq 9(2\sqrt{2} + 2C^*)\|G\|_{(L^2(D))^r} K_{\gamma,s}(\lambda)N^{-\frac{1}{s}},$$

(48)

with $g_i(\lambda)$ defined in (47),

$$K_{\gamma,s}(\lambda) := \left( \sum_{u \not\subseteq [s]} \gamma_u \prod_{i \in u} g_i(\lambda) \right)^{\frac{1}{s}} \left( \sum_{u \subseteq [s]} \left( \frac{|u|!^22^{|u|}}{\gamma_u} \prod_{i \in u} b_j \right)^2 \right)^{1/2}.$$ 

(49)

In general, $K_{\gamma,s}(\lambda)$ may grow with the parametric dimension $s$. In order to bound $K_{\gamma,s}(\lambda)$ uniformly with respect to $s \in \mathbb{N}$, we need to choose $\gamma_u$ carefully so that

$$K_{\gamma}(\lambda) := \left( \sum_{|u| < \infty} \gamma_u \prod_{i \in u} g_i(\lambda) \right)^{\frac{1}{s}} \left( \sum_{|u| < \infty} \left( \frac{|u|!^22^{|u|}}{\gamma_u} \prod_{i \in u} b_j \right)^2 \right)^{1/2} < \infty.$$ 

(50)

If (50) holds, then the estimate $K_{\gamma,s}(\lambda) \leq K_{\gamma}(\lambda) < \infty$ holds for any $s \in \mathbb{N}$, and accordingly the error bound (48) is independent of the dimension $s$.

**5.5 Choice of weight parameters $\gamma_u$**

For any $\lambda \in (1/2, 1]$, we follow the strategy in [34, 35] to choose weight parameters $\gamma_u$ that minimize the constant $K_{\gamma}(\lambda)$, cf. (50), and that $K_{\gamma}(\lambda)$ is finite. Note that the constant $K_{\gamma,s}(\lambda)$ in (49) and the uniform bound $K_{\gamma}(\lambda)$ in (50) have the same form.
as the function appearing in Lemma 18. Therefore, we can infer the proper form of the weight parameters \( \gamma_u \). Below we specify the parameter \( \lambda > 0 \) so that the constant \( K_\gamma(\lambda) \) is finite in our setting and to obtain a good convergence rate.

**Theorem 12.** Let \( \psi_j \) be the weight functions defined in (44) with \( a_j \) satisfying (45), and Assumption 3 hold for some \( p \leq 1 \). When \( p = 1 \), additionally, \( X_j \geq 1 \) if \( b_j \leq 1 \) and \( a_j \min \rho_{\max}(1) \) defined by replacing \( a_i \) in (47) by \( a_{\max} \) in (45). Then for each fixed \( \lambda \in (1/2, 1] \), the weight \( \gamma_u = \gamma^*_u(\lambda) := \left( (|u|!)^2 2^{2|u|} \prod_{j \in u} \frac{b_j^2}{a_j \rho_j(\lambda)} \right)^{1/(1+\lambda)} \) is the minimizer of \( K_\gamma(\lambda) \) if the minimum is finite. Additionally, if we choose

\[
\lambda = \lambda_* := \begin{cases} 
\frac{1}{2-\delta}, & \text{if } p \in (0, 2/3), \\
\frac{p}{2-p}, & \text{if } p \in (2/3, 1), \\
1, & \text{if } p = 1,
\end{cases}
\]

for arbitrary \( \delta \in (0, 1/2] \), and set \( \gamma_u = \gamma^*_u(\lambda_*) \), then \( K_\gamma(\lambda) < \infty \). Moreover, an RSLR can be constructed by a component-by-component algorithm such that

\[
\text{RMSE}_{\text{qmc}} \lesssim N^{-\chi}, \quad \text{with } \chi = (2\lambda_*)^{-1},
\]

where the constants are independent of the truncation dimension \( s \in \mathbb{N} \), but may depend on \( p \in (0, 1] \) and \( \delta \in (0, 1/2] \) if relevant.

**Proof.** First, note that the finite subsets of \( \mathbb{N} \) in (50) can be ordered and the specific choice of ordering is not important, since the convergence is unconditional. Therefore, by Lemma 18, the choice of weights (52) minimizes \( K_\gamma(\lambda) \), cf [34, 35]. Next, we prove that \( K_\gamma(\lambda) \) is finite when the weight and the parameter \( \lambda \) are given by (52) and (53), respectively. Indeed, define the following quantity

\[
S_\lambda := \sum_{|u| < \infty} (\gamma^*_u)^\lambda \prod_{j \in u} \rho_j(\lambda) = \sum_{|u| < \infty} \left( (|u|!)^2 2^{2|u|} \prod_{j \in u} \frac{[\rho_j(\lambda)]^{1/\lambda} b_j^2}{a_j} \right)^{1/(1+\lambda)}.
\]

Then \( K_\gamma(\lambda) = S_\lambda^{1/(2\lambda)+1/2} \), and hence it suffices to show that \( S_\lambda \) is finite. From (47), for each \( \lambda \), \( \rho_j(\lambda) \) monotonically increases with respect to \( a_j \), and thus we obtain \( \rho_j(\lambda) \leq \rho_{\max}(\lambda) \) for any \( j \geq 1 \). Consequently,

\[
S_\lambda \leq \sum_{|u| < \infty} \left( (|u|!)^2 2^{2|u|} \prod_{j \in u} \frac{4[\rho_{\max}(\lambda)]^{1/\lambda}}{a_{\min} b_j^2} \right)^{\lambda/(1+\lambda)}.
\]
Further, Assumption 3 also implies $a$ have \[(54). Since all terms in (54) are positive, it is sufficient to minimize each $\frac{4[\theta_{\max}(\lambda)]^{1/\lambda} b_j^2}{a_{\min}} A_j^{\lambda/(1+\lambda)}$ which is finite by assumption (51). This completes the proof of the theorem.

Then the constant $K_{\gamma}(\lambda)$ in (50) is minimized when $a_j = \sqrt{\frac{2\lambda - 1}{8\lambda}}$ for all $j \geq 1$.

Proof. In the proof of Theorem 12, we have $K_{\gamma}(\lambda) = S_\lambda^{1/(2\lambda) + 1/2}$, with $S_\lambda$ defined in (54). Since all terms in (54) are positive, it is sufficient to minimize each $\frac{4[\theta_{\max}(\lambda)]^{1/\lambda} b_j^2}{a_{\min}} A_j^{\lambda/(1+\lambda)}$ with respect to $a_j$, in order to minimize $K_{\gamma}(\lambda)$ with respect to $a_j$. By definition, we have $\left[\theta_j(\lambda)\right]^{1/\lambda} = \exp(a_j^2/\eta_j)$ for some $c > 0$ independent of $a_j$ and $\eta_j = \frac{1}{2} - \frac{1}{12\lambda}$. Then direct computation shows that the choice of $a_j$ minimizes $S_\lambda$, and hence $K_{\gamma}(\lambda)$. \qed
Theorem 14. Let the assumptions of Theorems 5, 6 and 12 hold. Then the RMSE of $Q_{s,N}(F^{j}_{s,h}; \Delta)$ with respect to the random shift $\Delta \in [0,1]^d$ is bounded by

$$
(\mathbb{E}^\Delta [(\mathbb{E}[\mathcal{G}(u(t_J))] - Q_{s,N}(F^{j}_{s,h}; \Delta))^2])^{1/2} \leq C(t_J^{1/2}h^2 + \tau + s^{-1/2 + \gamma} + N^{-\chi}),
$$

where the constant $C > 0$ is independent of positive parameters $h$, $\tau$, $s$ and $N$.

Proof. The error $\mathbb{E}[\mathcal{G}(u(t_J))] - Q_{s,N}(F^{j}_{s,h}; \Delta)$ can be decomposed into $\mathbb{E}[\mathcal{G}(u(t_J))] - \mathcal{G}(u^j_{s,h}) + \mathbb{E}[\mathcal{G}(u^j_{s,h}) - \mathcal{G}(u^{j+1}_{s,h})] + (\mathbb{E}[\mathcal{G}(u^{j+1}_{s,h})] - Q_{s,N}(F^{j+1}_{s,h}; \Delta))$, where the expectation $\mathbb{E}$ is with respect to $y \in U_b$. Then the desired bound on $(\mathbb{E}^\Delta [(\mathbb{E}[\mathcal{G}(u(t_J))] - Q_{s,N}(F^{j}_{s,h}; \Delta))^2])^{1/2}$ follows from Theorems 5, 6 and 12 directly. 

6 Numerical experiments

To complement the theoretical analysis, we present numerical results for the system (1)-(4) in the domain $[0,T] \times D \times \Omega$, with $T = 1$ and $D = (0,1)^2$. All computations were performed using MATLAB on HPC system at The University of Hong Kong, using 64 cores, each with 3GB memory.

In the computation, we take a time step size $\tau = 0.1$. We divide the square domain $D$ into $1/h^2$ congruent small squares (with $h = 1/16$), and then further divide each small square into two right triangles, obtaining a shape-regular triangulation $\mathcal{T}_h$. To solve problem (16), we employ the Taylor-Hood element on the mesh $\mathcal{T}_h$, i.e., a conforming piecewise quadratic element for the velocity $u$ and a conforming piecewise linear element for the pressure $p$. The resulting FEM spaces are given by

$$
H_h := \{W \in C(\overline{D})^2 : W|_K \in P_2(\overline{K})^2 \forall K \in \mathcal{T}_h \text{ and } W|_{\partial D} = 0\},
$$

$$
Q_h := \{\Pi \in C(\overline{D}) : \Pi|_K \in P_1(\overline{K}) \forall K \in \mathcal{T}_h \text{ and } \int_D \Pi \, dx = 0\}.
$$

This choice satisfies the discrete inf-sup condition (17). To handle the divergence-free subspace, we employ a continuous bilinear form $c(\cdot,\cdot)$ on $H_h \times Q_h$ by $c(v,q) = -\int_D q (\nabla \cdot v) \, dx$. The trilinear term $B[u,v,w]$, the Galerkin FEM scheme (19), arising from the convective term $(\mathbf{u} \cdot \nabla)\mathbf{u}$, is nonlinear. We employ Picard’s method to linearize the problem, which constructs a sequence of approximations $(u_{s,h}^{j+1,k},p_{s,h}^{j+1,k})$ by solving

$$
\begin{cases}
\tau^{-1}(u_{s,h}^{j+1,k} - u_{s,h}^j, v_h) + a(u_{s,h}^{j+1,k}, v_h) \\
\hspace{1cm} + B[u_{s,h}^{j+1,k-1}, u_{s,h}^{j+1,k}, v_h] + c(v_h, p_{s,h}^{j+1,k}) = 0, \quad \forall v_h \in H_h,
\end{cases}
$$

$$
c(u_{s,h}^{j+1,k}, q_h) = 0, \quad \forall q_h \in Q_h.
$$

This formulation is equivalent to the pressure-free formulation for the FEM approximation in Section 3, since we use an inf-sup stable velocity-pressure pair for the discrete solutions. We take the initialization $u_{s,h}^{1+1,0} = u_{s,h}^0$. The iteration process is
terminated when the relative $L^2(D)$-norm between the solutions of the current iteration and the previous one falls below a given tolerance $\eta = 10^{-7}$. Once the iteration converges after $K$ steps, we assign $u_{s,h}^{j+1} = u_{s,h}^{j+1,K}$ and $p_{s,h}^{j+1} = p_{s,h}^{j+1,K}$.

The random initial data $u_h^0$ is the $L^2(D)$-projection into $V_h$ of $u_0^0$, the truncated KL expansions with $s = 400$ of the initial condition $u^0$ in (5), which arises from the random field $Z$ with a zero mean and Matérn covariance function $\rho_\nu(|x - x'|)$, with $r = |x - x'|$ for all $x, x' \in D$, defined by

\[ \rho_\nu(r) = \sigma^2 \frac{2^{1 - \nu}}{\Gamma(\nu)} \left( \frac{2\sqrt{\nu} r}{\lambda_C} \right)^\nu K_\nu \left( \frac{2\sqrt{\nu} r}{\lambda_C} \right). \]

Here, $\Gamma$ is the Gamma function, $K_\nu$ is the modified Bessel function of the second kind, $\nu > 1/2$ is a smoothness parameter, $\sigma^2$ is the variance and $\lambda_C$ is a length scale parameter. Unlike the analysis, we conduct numerical tests without the smallness assumption in order to show the flexibility of the QMC method in a wider range of situations. Numerical results for initial data satisfying the smallness assumption are similar and hence not presented. Consider the Matérn covariance with the following parameter settings: $\nu = 2.5, 1.75$, $\lambda_C = 1, 0.1$, and $\sigma^2 = 1, 0.25$. We compute the eigenpairs of (11) on a finer mesh $T_h/4$ using conforming piecewise linear elements. The eigenpairs $(\mu_j, \xi_j)_{j=1}^s$ are used to construct $s$-term truncated KL expansions with $s = 400$, cf. Fig. 1. Additionally, we obtain the sequence $b = \{b_j\}_{j \geq 1}$ in (3) by utilizing the eigenpairs $(\mu_j, \xi_j)$. The summability parameter $p$ in Assumption 3 is estimated using linear regression on the sequence $|\log b_j|$ against $\log j$ for $500 \leq j \leq 1000$.

![Log-log plot of $|\xi_j|_{C_D}$, $|\nabla \xi_j|_{C_D}$ and $b_j$ against $j$ for the Matérn covariance with $\nu = 2.5$, $\sigma^2 = 1$ and $\lambda_C = 1$.](image)

Next, we use the component-by-component algorithm [33] to determine the generating vector $z \in Z^n$ for the RSLR with $N \in \mathbb{N}$ sampling points. To this end, we construct the weighted Sobolev space $W_h$ using the norm defined in (43). The weight parameters $\gamma_n$ are chosen according to (52), and the weight function $\psi^2(y)$ is defined
in (44). We select \( a_j = \sqrt{\frac{2\lambda_j - 1}{3\lambda_j}} \) based on (13), where the value of \( \lambda_j \) depends on the empirical estimate \( p \). We take \( R = 32 \) independent random shifts, cf. (32), where each sample \( \Delta_r \) for \( 1 \leq r \leq R \) is uniformly distributed over \([0,1]^R\). Then we use the generator vector \( z \in \mathbb{Z}^R \) to generate the \( N \) sampling points: \( (\frac{r}{N} + \Delta_r) \mod 1 \) for all \( 1 \leq i \leq N \). For the given quantity of interest defined by the linear functional \( \mathcal{G} \in (\mathcal{L}^2(\mathcal{D}))^\prime \), we compute the approximation \( Q_r := Q_{s,N}(F^{j,1}; \Delta_r) \) and its mean \( \bar{Q} \) over \( R \) random shifts, and obtain an unbiased estimator for the RMSE_qmc by \( \left( \frac{1}{R} \sum_{r=1}^{R} (Q_r - \bar{Q})^2 \right)^{1/2} \), i.e., the so-called standard error. We choose two bounded linear functionals \( \mathcal{G}_1 \) and \( \mathcal{G}_2 \); \( \mathcal{G}_1 \) evaluates the first component at the point \([1/2, 1/2]\) for \( t = 0.1 \), and \( \mathcal{G}_2 \) evaluates the second component at the same point for \( t = 0.2 \). We compute the standard errors \( e_1 \) and \( e_2 \) for \( \mathcal{G}_1 \) and \( \mathcal{G}_2 \), respectively.

First we take Matérn covariance with a smoothing parameter \( \nu = 2.5 \), a length scale parameter \( \lambda_C = 1 \) and a variance of \( \sigma^2 = 1 \) or \( \sigma^2 = 0.25 \). Numerically we observe that the sequence \( \{b_j\}^\infty_{j=1} \) lies under the \( \{j^{-3/2}\}^\infty_{j=1} \) for sufficiently large \( j \). Therefore, empirically, Assumption 3 holds with some \( p \leq 2/3 \), and thus we take \( \lambda_1 := 0.55 \) for these two cases. In Table 1, we compare the standard error of QMC with that of MC for the linear functionals \( \mathcal{G}_1 \) and \( \mathcal{G}_2 \). To obtain more precise estimates, for each number of sampling points \( N \), we use the mean of ten different tests with different uniformly distributed random shifts \( \Delta \) in (32). The rate of convergence is estimated by performing a linear regression of the negative logarithm of the standard error against \( \log N \), based on the mean of the ten tests. The results show that the QMC method yields a smaller error and a faster convergence rate for both cases. For instance, when the number of sampling points is \( N = 64007 \) and the variance is \( \sigma^2 = 1 \), the standard errors for the QMC and MC methods are \( 4.31 \times 10^{-5} \) and \( 1.81 \times 10^{-4} \), respectively. For the case of \( \lambda_C = 0.1 \), the empirical parameter \( p \) has the value of 0.6832, and hence we choose \( \lambda_1 = 0.52 \), which is presented in Table 2. The performance of the QMC method is similar to that observed in Table 1.

Table 1: Comparison of the standard error of QMC and MC with \( \mathcal{G}_1 \) and \( \mathcal{G}_2 \) for Matérn covariance with \( \nu = 2.5 \), \( \lambda_C = 1 \) and different \( \sigma^2 \).

<table>
<thead>
<tr>
<th>( N )</th>
<th>( \sigma^2 = 1 )</th>
<th>( \sigma^2 = 0.25 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>QMC</td>
<td>MC</td>
</tr>
<tr>
<td>1009</td>
<td>6.36e-4</td>
<td>4.65e-5</td>
</tr>
<tr>
<td>2003</td>
<td>3.77e-4</td>
<td>6.00e-5</td>
</tr>
<tr>
<td>4001</td>
<td>3.79e-4</td>
<td>5.80e-5</td>
</tr>
<tr>
<td>8009</td>
<td>1.79e-4</td>
<td>3.03e-5</td>
</tr>
<tr>
<td>16001</td>
<td>1.23e-4</td>
<td>1.12e-5</td>
</tr>
<tr>
<td>32003</td>
<td>6.24e-5</td>
<td>1.20e-5</td>
</tr>
<tr>
<td>64007</td>
<td>4.31e-5</td>
<td>7.90e-6</td>
</tr>
<tr>
<td>Rate</td>
<td>0.66</td>
<td>0.52</td>
</tr>
</tbody>
</table>

Next, we consider Matérn covariance with a smoothing parameter \( \nu = 1.75 \) and length scale parameter \( \lambda_C = 1 \) or \( \lambda_C = 0.1 \), with variances of \( \sigma^2 = 1 \) or \( \sigma^2 = 0.25 \),
Table 2: Comparison of the standard error of QMC and MC with $G_1$ and $G_2$ for Matérn covariance with $\nu = 2.5$, $\lambda_C = 0.1$ and different $\sigma^2$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\sigma^2 = 1$</th>
<th>$\sigma^2 = 0.25$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>MC $e_1$ $e_2$</td>
</tr>
<tr>
<td></td>
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<td>MC $e_1$ $e_2$</td>
</tr>
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</tr>
<tr>
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<td>3.37e-3 1.33e-4</td>
</tr>
<tr>
<td>8009</td>
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<td>1.53e-3 1.31e-4</td>
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<tr>
<td>16001</td>
<td>2.18e-4 1.96e-5</td>
<td>1.30e-3 6.77e-5</td>
</tr>
<tr>
<td>32003</td>
<td>1.66e-4 1.03e-5</td>
<td>7.29e-4 5.10e-5</td>
</tr>
<tr>
<td>64007</td>
<td>9.53e-5 8.67e-6</td>
<td>7.14e-4 4.33e-5</td>
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</table>

<table>
<thead>
<tr>
<th>Rate</th>
<th>0.68</th>
<th>0.58</th>
<th>0.36</th>
<th>0.41</th>
</tr>
</thead>
</table>

Table 3: Comparison of the standard error of QMC and MC with $G_1$ and $G_2$ for Matérn covariance with $\nu = 1.75$, $\lambda_C = 1$ and different $\sigma^2$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\sigma^2 = 1$</th>
<th>$\sigma^2 = 0.25$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>QMC $e_1$ $e_2$</td>
<td>MC $e_1$ $e_2$</td>
</tr>
<tr>
<td></td>
<td>QMC $e_1$ $e_2$</td>
<td>MC $e_1$ $e_2$</td>
</tr>
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</tr>
<tr>
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<td>1.39e-3 1.42e-4</td>
</tr>
<tr>
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<td>2.93e-4 3.85e-5</td>
<td>7.29e-4 8.35e-5</td>
</tr>
<tr>
<td>8009</td>
<td>1.78e-4 2.85e-5</td>
<td>5.14e-4 7.16e-5</td>
</tr>
<tr>
<td>16001</td>
<td>1.91e-4 1.78e-5</td>
<td>5.12e-4 5.37e-5</td>
</tr>
<tr>
<td>32003</td>
<td>1.15e-4 1.03e-5</td>
<td>5.90e-4 3.70e-5</td>
</tr>
<tr>
<td>64007</td>
<td>6.77e-5 6.08e-6</td>
<td>3.29e-4 2.67e-5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Rate</th>
<th>0.53</th>
<th>0.65</th>
<th>0.37</th>
<th>0.50</th>
</tr>
</thead>
</table>

Finally, we summarize all the numerical experiments from Table 1 to Table 4 and illustrate their convergence in Fig. 2 and Fig. 3. The results clearly demonstrate that our proposed QMC method outperforms the MC method in terms of the standard error for all cases. Additionally, the QMC method exhibits a faster convergence rate compared to the MC method in most cases. These findings validate the effectiveness of the proposed QMC approach for solving the given problem.
Table 4: Comparison of the standard error of QMC and MC with $G_1$ and $G_2$ for Matérn covariance with $\nu = 1.75$, $\lambda_C = 0.1$ and different $\sigma^2$.

<table>
<thead>
<tr>
<th>$\sigma^2$</th>
<th>$\nu = 1.75$</th>
<th>$\nu = 0.1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_C$</td>
<td>$\sigma^2 = 1$</td>
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<tr>
<td>$\sigma^2 = 1$</td>
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<td>MC</td>
</tr>
<tr>
<td>N</td>
<td>$\epsilon_1$</td>
<td>$\epsilon_2$</td>
</tr>
<tr>
<td>1009</td>
<td>1.76e-3</td>
<td>9.78e-5</td>
</tr>
<tr>
<td>2003</td>
<td>7.76e-4</td>
<td>7.40e-5</td>
</tr>
<tr>
<td>4001</td>
<td>3.78e-4</td>
<td>3.73e-5</td>
</tr>
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<td>8009</td>
<td>4.54e-4</td>
<td>5.60e-5</td>
</tr>
<tr>
<td>16001</td>
<td>9.48e-5</td>
<td>1.50e-5</td>
</tr>
<tr>
<td>32003</td>
<td>9.23e-5</td>
<td>8.54e-6</td>
</tr>
</tbody>
</table>

| Rate | 0.72 | 0.69 | 0.47 | 0.44 | 0.81 | 0.73 | 0.46 | 0.44 |

Fig. 2: The standard errors of $\epsilon_1$ with various Matérn covariance parameters for QMC and MC plotted versus the number of sampling points $N$. 

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Fig. 3: The standard errors of $\varepsilon_2$ with various Matérn covariance parameters for QMC and MC plotted versus the number of sampling points $N$.

7 Conclusion

In this paper, we have investigated the Navier-Stokes equations with random initial data in a bounded polygonal domain $D \subset \mathbb{R}^2$. We have developed a scheme for approximating the expected value of the solution, by combining Galerkin FEM, truncated Karhunen-Loève expansion of the log-normal initial random field, and quasi-Monte Carlo (QMC) method. Further, we have derived a bound on the root-mean-square error, including the finite element error, the dimension truncation error, and the error from the QMC quadrature. The numerical experiments show that the scheme enjoys fast convergence with respect to the number of sampling points. To the best of our knowledge, this work represents the first theoretical QMC analysis for nonlinear PDEs.
Theoretically, it is of interest to extend the analysis to a more general class of PDEs. Of particular interest are non-Newtonian fluid flow models, describing the motion of fluids with a more general structure \[19, 20\]. The extension requires a new way to control the fully non-linear diffusion term, and a more refined analysis for the convective term. From an algorithmic point of view, it is of much interest to consider the multilevel and/or changing dimension algorithms \[36–39\], with the QMC algorithm applied to the PDE problems with random data \[40–43\]. Adapting these algorithms to the Navier–Stokes problem is an intriguing topic.

**Acknowledgements**

GL acknowledges the support from Young Scientists fund (Project number: 12101520) by NSFC and GRF (project number: 17317122), RGC, Hong Kong.

**Appendix A Useful inequalities**

In this appendix we collect several useful inequalities. We use Ladyzhenskaya’s inequality \[6, Lemma 3.3\] frequently.

**Lemma 15.** For any open set \(D \subset \mathbb{R}^2\), the following inequality holds
\[
\|u\|_{L^4(D)} \leq 2^{1/4} \|u\|_{L^2(D)}^{1/2} \|\nabla u\|_{L^2(D)}^{1/2}, \quad \forall u \in H_0^1(D)^2.
\]  

(A1)

We also need the following discrete Gronwall inequality \[15, Lemma 5.1\].

**Lemma 16.** Let the non-negative numbers \(k, B\) and \(a_j, b_j, c_j, \gamma_j\) satisfy
\[
a_n + k \sum_{j=0}^{n} b_j \leq k \sum_{j=0}^{n} \gamma_j a_j + k \sum_{j=0}^{n} c_j + B, \quad \text{for all } n \geq 0. \quad \text{If } k \gamma_j < 1 \text{ for all } j \geq 0, \text{ then}
\]
\[
a_n + k \sum_{j=0}^{n} b_j \leq \left( k \sum_{j=0}^{n} c_j + B \right) \exp \left( k \sum_{j=0}^{n} \gamma_j \right), \quad \forall n \geq 0.
\]

We also need the following version of Fernique’s theorem \[
].

**Theorem 17.** Let \(E\) be a real separable Banach space and \(X\) be an \(E\)-valued and centered Gaussian random variable, in the sense that, for each \(x^* \in E^*\), \(\langle X, x^* \rangle\) is a centered, real-valued Gaussian random variable. Then with \(R := \inf\{r \in [0, \infty) : P(\|X\|_E \leq r) \geq \frac{3}{4}\}\), \(\int_{\Omega} \exp \left( \frac{\|X\|_E^2}{2R^2} \right) dP(\omega) \lesssim 1\).

Last, we recall the following two auxiliary lemmas \[34, 35\].

**Lemma 18.** Fix \(m \in \mathbb{N}, \lambda > 0\) and \(A_i, B_i > 0\) for all \(i \in \mathbb{N}\). Then the quantity
\[
\left( \sum_{i=1}^{m} x_i A_i \right)^{1/4} \left( \sum_{i=1}^{m} \frac{B_i}{x_i} \right)
\]

is minimized over any sequences \((x_i)_{1 \leq i \leq m}\) when
\[
x_i = c (B_i/A_i)^{1/4} \quad \text{for all } c > 0.
\]

(A3)
For $m \to \infty$, the function \((A2)\) is minimized provided that $x_i$ is defined by \((A3)\) for each $i$ and it is finite if and only if $\sum_{i=1}^{\infty} (A_iB_i^{\lambda})^{1/(1+\lambda)}$ converges.

**Lemma 19.** Fix $A_j > 0$ for all $j \in \mathbb{N}$ and $\sum_{j=1}^{\infty} A_j < 1$. Then we have

$$\sum_{|u| < \infty} |u|! \prod_{j \in u} A_j \leq \sum_{k=0}^{\infty} \left( \sum_{j \geq 1} A_j \right)^k = \frac{1}{1 - \sum_{j \geq 1} A_j}.$$

Furthermore, for any $B_j > 0$ with $\sum_{j=1}^{\infty} B_j < \infty$, we also have

$$\sum_{|u| < \infty} \prod_{j \in u} B_j = \prod_{j \geq 1} (1 + B_j) = \exp \left( \sum_{j \geq 1} \log(1 + B_j) \right) \leq \exp \left( \sum_{j \geq 1} B_j \right).$$

**References**


[33] Nichols, J., Kuo, F.: Fast CBC construction of randomly shifted lattice rules achieving \( O(n^{-1+\delta}) \) convergence for unbounded integrands over \( \mathbb{R}^s \) in weighted spaces with POD weights. J. Complexity 30(4), 444–468 (2014) https://doi.org/10.1016/j.jco.2014.02.004

[34] Kuo, F., Schwab, C., Sloan, I.: Quasi-Monte Carlo finite element methods for a


