RAPID COVARIANCE-BASED SAMPLING OF LINEAR SPDE APPROXIMATIONS IN THE MULTILEVEL MONTE CARLO METHOD

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Abstract. The efficient simulation of the mean value of a non-linear functional of the solution to a linear stochastic partial differential equations (SPDE) with additive Gaussian noise at a fixed time is considered. A Galerkin finite element method is employed along with an implicit Euler scheme to arrive at a fully discrete approximation of the mild solution to the equation. A scheme is presented to compute the covariance of this approximation, which allows for rapid sampling in a Monte Carlo method. This is then extended to a multilevel Monte Carlo method (MLMC), for which a scheme to compute the cross-covariance between the approximations at different levels is presented. In contrast to traditional path-based methods it is not assumed that the Galerkin subspaces at these levels are nested. The computational complexities of the presented schemes are compared to traditional methods and simulations confirm that the costs of the latter are significantly greater than those of the former.

1. Introduction

Stochastic partial differential equations (SPDE) have many applications in engineering, finance, biology and meteorology. These include filtering problems, pricing of energy derivative contracts and modeling rare climate phenomena. For an overview of applications we refer to [6, 13]. A natural quantity of interest for an SPDE is the expected value of a non-linear functional of the solution of the equation at a fixed time, including moments of it. In order to determine such quantities, numerical approximations of the SPDE have to be considered, since analytical solutions are in general unavailable.

The field of numerical analysis of SPDE is a very active one and a multitude of approximations have been considered in the literature, see e.g., [9] for an overview of such approximations. In this paper we take the approach of [10], where the author considers an SPDE of evolutionary type and employs a Galerkin method for the spatial discretization of the equation (which includes both spectral and finite element methods) along with a backward Euler-Maruyama scheme for the temporal discretization. The finite element method in particular is useful and flexible as no explicit knowledge of eigenfunctions or eigenvalues is needed. The author of [10] does, however, omit the problem of how to, given this approximation, efficiently estimate expected values, and this is the question we are concerned with in this paper.

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Typically, the approximation of expected values is accomplished by a Monte Carlo method, i.e., by computing a large number of sample paths of the approximate solution and taking the average of the functional of interest applied to each of them. This is however quite expensive. Starting with the publication of [7], in turn inspired by earlier work, the multilevel Monte Carlo method (MLMC) has become popular, since it can reduce the computational complexity of this problem. We refer to [8] for an introduction to this rapidly developing field and to [3] and [4] for applications of the multilevel Monte Carlo method to finite element approximations of SPDE.

Even though the multilevel Monte Carlo method decreases the computational cost of the approximation of expected values, it is still fairly expensive. The idea of this paper is to exploit the fact that as long as the SPDE we consider has additive noise and is (affine) linear, then the approximation from [10] of the end-time solution is Gaussian. Since a Gaussian random variable is completely determined by its mean and covariance, calculating these parameters provides an efficient way of sampling the approximation. We also show how to incorporate this idea in a multilevel Monte Carlo method by calculating the cross-covariance between two SPDE approximations in different Galerkin subspaces. In contrast to [3] and [4], we do not assume that the Galerkin subspace sequence is nested.

The paper is organized as follows: In Section 2 we recapitulate the theoretical setting and approximation results of [10]. We also mention some theoretical results that we will make use of and we give a concrete example of an SPDE that fulfills the assumptions we make on the parameters of the equation. In Section 3 we introduce a covariance-based method for computing samples of SPDE approximations in a Monte Carlo setting and compare the complexity of it to the traditional path-based method. We extend this in Section 4 to the setting of the multilevel Monte Carlo method. Finally in Section 5 we demonstrate the efficiency of our approach by simulation of the stochastic heat equation.

2. SPDE setting

Let $H$ be a real separable Hilbert space with inner product $\langle \cdot, \cdot \rangle$ and induced norm $\| \cdot \|$ and let $-A: \text{dom}(-A) \subset H \rightarrow H$ be a positive definite, self-adjoint operator with a compact inverse on $H$. For $0 < T < \infty$, let $(\Omega, \mathcal{A}, (\mathcal{F}_t)_{t \in [0,T]}, P)$ be a complete filtered probability space satisfying the usual conditions, which is to say that $\mathcal{F}_0$ contains all $P$-null sets and $\mathcal{F}_t = \cap_{s > t} \mathcal{F}_s$ for all $t \in [0,T]$. In this context we consider the linear SPDE

$$dX(t) = (AX(t) + F(t, X(t))) \, dt + G(t) \, dW(t),$$

$$X(0) = x_0,$$

(1)

for $t \in [0,T]$. Here $W$ is an $H$-valued $Q$-Wiener process, $x_0$ is a random member of a subspace of $H$, while $F$ and $G$ are mappings that fulfill Assumption 2.1 below. The solution $X = (X(t))_{t \in [0,T]}$ is then an $H$-valued stochastic process. Equation (1) is treated with the semigroup approach of [6, Chapter 7], resulting in a so called mild solution of the equation. In order to introduce this notion, we start by introducing the spectral structure induced by $A$ on $H$.

By the spectral theorem applied to $(-A)^{-1}$ we get an orthonormal eigenbasis $(e_i)_{i \in \mathbb{N}}$ of $H$ and a positive sequence $(\lambda_i)_{i \in \mathbb{N}}$ of eigenvalues of $-A$ that is increasing and for which
\[ (-A)^{\frac{\lambda}{2}} f = \sum_{i=1}^{\infty} \lambda_i^\frac{\lambda}{2} \langle f, e_i \rangle e_i \]

for \( f \in \dot{H}^r = \text{dom}(\dot{(-A)^{\frac{\lambda}{2}}}) \), which is characterized by

\[
\dot{H}^r = \left\{ f = \sum_{i=1}^{\infty} f_i e_i : f_i \in \mathbb{R} \text{ for all } i \in \mathbb{N} \text{ and } \|f\|^2_{\dot{H}^r} = \sum_{i=1}^{\infty} \lambda_i^r f_i^2 < \infty \right\}.
\]

This is a separable Hilbert space when equipped with the inner product

\[
\langle \cdot, \cdot \rangle_r = \left\langle (-A)^{\frac{\lambda}{2}}, (-A)^{\frac{\lambda}{2}} \right\rangle.
\]

Note that for \( r > 0 \), we have the Gelfand triple \( H^r \subseteq \dot{H} \subseteq H^{-r} \) since \( H^{-r} \cong (\dot{H}^r)' \), the dual of \( \dot{H}^r \). The operator \( A \) is furthermore the generator of a strongly continuous semigroup \( E = (E(t))_{t \geq 0} \) of linear operators on \( H \).

Next, we briefly recapitulate some important notions from functional analysis and probability theory that we need. For two real separable Hilbert spaces \( H_1 \) and \( H_2 \), we denote by \( H_1 \oplus H_2 = \{ [f, u] : f \in H_1, u \in H_2 \} \) the Hilbert (external) direct sum of \( H_1 \) and \( H_2 \). With an inner product defined by \( \langle [f_1, u_1']', [f_2, u_2'] \rangle_{H_1 \oplus H_2} = \langle f_1, f_2 \rangle_{H_1} + \langle u_1, u_2 \rangle_{H_2} \), \( f_1, f_2 \in H_1, u_1, u_2 \in H_2 \), this is indeed a Hilbert space. Similarly, by \( H_1 \otimes H_2 \) we denote the Hilbert tensor product, i.e., the completion of the algebraic tensor product of \( H_1 \) and \( H_2 \) under the norm induced by the inner product \( \langle f_1 \otimes u_1, f_2 \otimes u_2 \rangle_{H_1 \otimes H_2} = \langle f_1, f_2 \rangle_{H_1} \langle u_1, u_2 \rangle_{H_2} \), \( f_1, f_2 \in H_1, u_1, u_2 \in H_2 \). For \( H_1 = H_2 \) we use the notation \( H_1^\otimes 2 = H_1 \otimes H_1 \) and \( f \otimes f \) for \( f \in H_1 \).

We denote by \( \mathcal{L}(H_1, H_2) \) and \( \mathcal{L}(H_1, H_2) \), or \( \mathcal{L}(H) \) respectively \( \lambda_2(H) \) when \( H_1 = H_2 = H \), the spaces of linear respectively Hilbert-Schmidt operators from \( H_1 \) to \( H_2 \). The latter is defined by

\[
\mathcal{L}_2(H_1, H_2) = \{ K \in \mathcal{L}(H_1, H_2) : \sum_{i=1}^{\infty} \|Ke_i\|^2_{H_2} < \infty \}
\]

where \((e_i)_{i \in \mathbb{N}}\) is an arbitrary orthonormal basis of \( H_1 \). Similarly, the family of trace class operators on \( H \) is defined by

\[
\mathcal{L}_1(H) = \{ K \in \mathcal{L}(H) : \text{Tr}(K) = \sum_{i=1}^{\infty} \langle Ke_i, e_i \rangle^2 < \infty \}.
\]

For an \( H \)-valued random variable \( X \), the expected value, or mean, of \( X \) is defined by the Bochner integral

\[
\mathbb{E}[X] = \int_{\Omega} X(\omega) \, dP(\omega),
\]

which is well defined if \( X \in L^1(\Omega; H) \), i.e., if \( \mathbb{E}\|X\| < \infty \). If \( X \in L^2(\Omega; H) \), we define the covariance or covariane operator of \( X \) by

\[
\text{Cov}(X) = \mathbb{E}[(X - \mathbb{E}[X]) \otimes (X - \mathbb{E}[X])] = \mathbb{E}[X \otimes X] - \mathbb{E}[X] \otimes \mathbb{E}[X] \in H \otimes 2.
\]

More generally, for Hilbert spaces \( H_1 \) and \( H_2 \), we define the cross-covariance or cross-covariance operator of an \( H_2 \)-valued random variable \( Y \in L^2(\Omega; H_2) \) and an \( H_1 \)-valued random variable \( Z \in L^2(\Omega; H_1) \) by

\[
\text{Cov}(Y, Z) = \mathbb{E}[(Y - \mathbb{E}[Y]) \otimes (Z - \mathbb{E}[Z])] = \mathbb{E}[Y \otimes Z] - \mathbb{E}[Y] \otimes \mathbb{E}[Z] \in H_2 \otimes H_1.
\]
so that $\text{Cov}(X) = \text{Cov}(X, X)$. Calling these quantities operators is justified by the fact that $H_2 \otimes H_1 \simeq \mathcal{L}_2(H_1, H_2) \subseteq \mathcal{L}(H_1, H_2)$. The action of the cross-covariance is given by $\text{Cov}(Y, Z) = \mathbb{E}((Z - \mathbb{E}[Z], \cdot)_{H_1} (Y - \mathbb{E}[Y]))$ and from this we have $\text{Tr}(\text{Cov}(X)) = \mathbb{E}[\|X - \mathbb{E}[X]\|_H^2] < \infty$, i.e., the covariance operator of a random variable $X \in L^2(\Omega; H)$ is of trace class, and also that $\text{Cov}(X)$ is a self-adjoint operator that is positive semidefinite, which implies that it has a unique square root.

We next recall that an $H$-valued random variable $X$ is said to be Gaussian if $X \in H$ $\mathbb{P}$-a.s. and $(X, f)$ is a real-valued Gaussian random variable for all $f \in H$. In this case $X \in L^p(\Omega; H)$ for all $p \geq 1$ so $\text{Cov}(X)$ is well-defined. Now, a stochastic process $W : [0, T] \times \Omega \to H$ is said to be an $H$-valued Q-Wiener process adapted to $(\mathcal{F}_t)_{t \in [0, T]}$ if $W(0) = 0$, $W$ has $\mathbb{P}$-a.s. continuous trajectories, and if there exists a self-adjoint trace class operator $Q \in \mathcal{L}(H)$ such that for each $0 \leq s < t \leq T$, $W(t) - W(s)$ is Gaussian with zero mean and covariance $(t-s)Q$ and $W(t) - W(s)$ is independent of $\mathcal{F}_s$. For more details on Hilbert space-valued Gaussian random variables and Wiener processes we refer to [6, Chapters 2-4].

With these notions in mind, a predictable process $X = (X(t))_{t \in [0, T]}$ is called a mild solution to (1) if

$$\sup_{t \in [0, T]} \|X(t)\|_{L^2(\Omega; H)} < \infty$$

and for all $t \in [0, T]$,

$$X(t) = E(t)x_0 + \int_0^t E(t-s)F(s, X(s)) \, ds + \int_0^t E(t-s)G(s) \, dW(s), \quad \mathbb{P}\text{-a.s.}$$

Here the first integral is of Bochner type while the second is an $H$-valued Itô-integral, the construction of which is found in [6, Chapter 4]. For this to be well defined, we need to map $G$ to $\mathcal{L}_2^0 = \mathcal{L}_2(Q^{1/2}(H), H)$. Here $Q^{1/2}(H)$ is a Hilbert space equipped with the inner product $\langle Q^{1/2}, Q^{-1/2} \rangle$, where $Q^{-1/2}$ denotes the pseudo-inverse of $Q^{1/2}$. We make this explicit in the assumption below, which is a stronger version of the assumptions needed for [10, Theorem 2.25] to guarantee the existence of a mild solution to (1). It also guarantees that the approximation to the mild solution SPDE (1) that we consider below is Gaussian.

**Assumption 2.1.** The parameters of the SPDE (1) fulfill the following requirements.

(i) For an operator $Q \in \mathcal{L}(H)$ that is of trace class, self-adjoint and positive semidefinite, $W = (W(t))_{t \in [0, T]}$ is a $Q$-Wiener process adapted to $(\mathcal{F}_t)_{t \in [0, T]}$.

(ii) There exists a constant $C$ such that $G : [0, T] \to \mathcal{L}_2^0$ satisfies

$$\|G(t_1) - G(t_2)\|_{\mathcal{L}_2^0} \leq C|t_1 - t_2|^{1/2}$$

for all $t_1, t_2 \in [0, T]$.

(iii) The function $F : [0, T] \times H \to \dot{H}^{-1}$ is affine in $H$, i.e., for each $t \in [0, T]$ there exists an operator $F_t^1 \in \mathcal{L}(H, \dot{H}^{-1})$ and an element $F_t^2 \in \dot{H}^{-1}$ such that $F(t, f) = F_t^1 f + F_t^2$ for all $f \in H$. Furthermore, there exists a constant $C$ such that $F : [0, T] \times H \to \dot{H}^{-1}$ satisfies

$$\|F(t_1, f) - F(t_2, f)\|_{-1} \leq C(1 + \|f\|)|t_1 - t_2|^{1/2}$$

for all $f \in H$, $t_1, t_2 \in [0, T]$, and $\|F_t^2\|_{\mathcal{L}(H, \dot{H}^{-1})} \leq C$ for all $t \in [0, T]$.

(iv) The initial value $x_0$ is a (possibly degenerate) $\mathcal{F}_0$-measurable $\dot{H}^1$-valued Gaussian random variable.
Since \( x_0 \in L^p(\Omega; H) \) for all \( p \geq 1 \) and the rest of the parameters of (1) are assumed to be deterministic, this assumption also guarantees that

\[
\sup_{t \in [0,T]} \|X(t)\|_{L^p(\Omega; \dot{H}^s)} < \infty
\]

for all \( p \geq 1 \) and \( s \in [0,1) \).

As a model problem in this context, we consider a stochastic advection-diffusion equation.

**Example 2.2.** For a convex polygonal domain \( D \subset \mathbb{R}^d \), \( d = 1, 2, 3 \), let \( H = L^2(D) \) and for a function \( f \) on \( D \), let the operator \(-A\): \( \text{dom}(-A) \rightarrow H \) be given by \( Af = \nabla \cdot (a \nabla f) \) with Dirichlet zero boundary conditions, where \( a : D \rightarrow \mathbb{R} \) is a sufficiently smooth strictly positive function. In this setting it holds (cf. [16, Chapter 3]) that \( \dot{H}^1 = H^1_0(D) \) and \( \dot{H}^2 = H^2(D) \cap H^1_0(D) \), where \( H^k(D) \) is the Sobolev space of order \( k \) on \( D \) and \( H^1_0(D) \) consists of those functions in \( H^1(D) \) that are zero on the boundary \( \partial D \) of \( D \). Let \( F \) be a convection term given by \( F(t,f) = b(t,\cdot) \cdot \nabla f(\cdot) \) for a function \( f \) on \( D \). Provided that the vector field \( b : D \times [0,T] \rightarrow \mathbb{R}^d \) is smooth enough, \( F(t,\cdot) \) is indeed a member of \( \mathcal{L}(H, \dot{H}^{-1}) \) (cf. [10, Example 2.22]). Choosing \( G = I \) and \( x_0 \) smooth enough, Equation (1) is interpreted as the problem to find a function-valued stochastic process \( X \) such that

\[
dX(t,x) = (\nabla \cdot (a(x)\nabla X(t,x)) + b(t,x) \cdot \nabla X(t,x)) \, dt + dW(t,x) \quad \text{for all } t \in (0,T], \, x \in D,
\]

where the space derivatives should be understood as weak derivatives of Sobolev spaces. Furthermore, the noise term has a more concrete meaning in this setting of \( H = L^2(D) \). A consequence of \( \text{Tr}(Q) < \infty \) is that \( Q^{1/2} \in \mathcal{L}_2(H) \). Therefore, by [14, Proposition A.7] (see also [6, Section 4.1.3]), there exists a symmetric square integrable function \( q : D \times D \rightarrow \mathbb{R} \) such that

\[
Qf = \int_D q(\cdot,y)f(y) \, dy
\]

for \( f \in H \). Similarly, if \( q \) is a symmetric, positive semidefinite continuous function on \( D \times D \), then (2) defines a covariance operator by [14, Theorem A.8]. If we take \( W(t,\cdot) \), \( t \in [0,T] \), to be a random field (which in this setting is to say that it is defined in all of \( D \) and jointly \( \mathcal{B}(D) \otimes \mathcal{F}_t \)-measurable, where \( \mathcal{B}(D) \) denotes the Borel \( \sigma \)-algebra on \( D \)) then it is easily seen that \( tq \) coincides with the covariance function of the field.

For the spatial discretization of (1), we assume the setting of [10, Chapter 3.2]. We let \((V_h)_{h \in (0,1]}\) be a family of subspaces of \( \dot{H}^1 \) equipped with the inner product of \( H \) such that \( N_h = \dim(V_h) < \infty \), \( h \in (0,1] \). By \( P_h : \dot{H}^{-1} \rightarrow V_h \) we denote the generalized orthogonal projector onto \( V_h \) with respect to the inner product of \( H \), which is defined by

\[
\langle P_h f, \Phi \rangle = \langle A^{-1} f, \Phi \rangle_1
\]

for all \( f \in \dot{H}^{-1} \) and \( \Phi \in V_h \). We assume that for the given family there exists a constant \( C \) such that \( \|P_h x\|_1 \leq C\|x\|_1 \) and \( \|R_h x - x\| \leq C\|x\|_h h^s \) for all \( h \in (0,1] \) and all \( x \) in \( \dot{H}^1 \) and \( \dot{H}^s \), \( s \in (0,1] \), respectively. Here \( R_h \) is the Ritz projector, i.e., the orthogonal projector \( R_h : \dot{H}^1 \rightarrow V_h \) with respect to the inner product \( \langle \cdot, \cdot \rangle_1 \) in \( \dot{H}^1 \). With this framework both
finite element and spectral methods are included (cf. [10, Example 3.6-3.7]). The operator 
\[-A_h : V_h \to V_h,\] is now defined by the relationship 
\[
(A_h f_h, g_h) = \langle f_h, g_h \rangle_1 = \left< (-A)^{\frac{1}{2}} f_h, (-A)^{\frac{1}{2}} g_h \right>
\]
for all \( f_h, g_h \in V_h. \) For the temporal discretization, we use the backward Euler method. 
Let us take a uniform time grid given by \( t_j = j \Delta t \) for \( j = 0, \ldots, N_{\Delta t} \), where \( N_{\Delta t} \in \mathbb{N} \) and \( \Delta t = TN_{\Delta t}^{-1}. \) A fully discrete approximation \((X_{h,\Delta t}^{t_j})_{j=0}^{N_{\Delta t}}\) is then given by the recursion
\[
X_{h,\Delta t}^{t_{j+1}} - X_{h,\Delta t}^{t_j} = \left( A_h X_{h,\Delta t}^{t_j} + P_h F(t_j, X_{h,\Delta t}^{t_j}) \right) \Delta t + P_h G(t_j) \Delta W_j,
\]
where \( \Delta W_j = W(t_{j+1}) - W(t_j) \) and \( j = 0, \ldots, N_{\Delta t} - 1. \) It converges strongly to the solution
of (1) in the sense of the following theorem.

**Theorem 2.3.** [10, Theorem 3.14] Let the terms of the (1) satisfy Assumption 2.1 and let 
\((X_{h,\Delta t}^{T})_{h,\Delta t}\) be a family of fully discrete approximations of \( X(T) \) given by the backward Euler scheme (3). Then, for all \( p \geq 1, \) \( \sup_{h,\Delta t} \|X_{h,\Delta t}^{T}\|_{L^p(\Omega; H)} < \infty \) and there exists a constant \( C > 0 \) such that, for all \( h, \Delta t \in (0,1], \)
\[
\|X(T) - X_{h,\Delta t}^{T}\|_{L^p(\Omega; H)} \leq C \left( h + \Delta t^{1/2} \right).
\]

Recalling that the goal is the approximation of the quantity \( \mathbb{E}[\phi(X(T))] \), the concept of weak convergence is vital, as it allows us to tune the Monte Carlo estimators of Sections 3
and 4. In order to use the weak convergence result of [10], we need stronger assumptions on \( F \) and \( G. \) This is formalized in the next assumption, along with an assumption on \( \phi. \)

**Assumption 2.4.** The parameters of the SPDE (1) fulfill, for some \( \delta \in [1/2,1], \) the following requirements.

(i) There exists a constant \( C \) such that \( G : [0,T] \to \mathcal{L}_2^0 \) satisfies
\[
\|G(t_1) - G(t_2)\|_{\mathcal{L}_2^0} \leq C|t_1 - t_2|^{\delta}
\]
for all \( t_1, t_2 \in [0,T]. \)

(ii) There exists a constant \( C \) such that \( F : [0,T] \to H \) satisfies
\[
\|F(t_1) - F(t_2)\| \leq C|t_1 - t_2|^{\delta}
\]
for all \( f \in H, t_1, t_2 \in [0,T]. \)

Furthermore, the functional \( \phi : H \to \mathbb{R} \) is a member of \( C_2^0(H; \mathbb{R}), \) the space of all continuous mappings from \( H \) to \( \mathbb{R} \) which are 2 times continuously Fréchet-differentiable such that its 
derivatives are at most polynomially growing.

With this assumption in place in place, we cite the following weak convergence result.

**Theorem 2.5.** [10, Theorem 5.12] Let \( \phi \) and the terms of (1) satisfy Assumptions 2.1 and
2.4, let \((X_{h,\Delta t}^{T})_{h,\Delta t} \) and \( X(T) \) be as in Theorem 2.3. Then there exists a constant \( C > 0 \) such 
that, for all \( h, \Delta t \in (0,1], \)
\[
\left| \mathbb{E} \left[ \phi(X(T)) - \phi(X_{h,\Delta t}^{T}) \right] \right| \leq C \left( 1 + |\log(h)| \right) \left( h^2 + \Delta t^{\delta} \right).
\]
3. Covariance-based sampling in a Monte Carlo setting

The Monte Carlo approximation of $E[Y]$, where $Y$ is a real-valued random variable, is given by

$$E_N[Y] = \frac{1}{N} \sum_{i=1}^{N} Y^{(i)},$$

where $N \in \mathbb{N}$ is the number of independent realizations, $Y^{(i)}$, of $Y$. By [4, Lemma 4.1] we have that for $Y \in L^2(\Omega;\mathbb{R})$ and $N \in \mathbb{N}$,

$$\| E[Y] - E_N[Y] \|_{L^2(\Omega;\mathbb{R})} \leq \frac{1}{\sqrt{N}} \text{Var}(Y) \leq \frac{1}{\sqrt{N}} \| Y \|_{L^2(\Omega;\mathbb{R})}.$$

In order to accurately approximate $E[\phi(X(T))]$ by a Monte Carlo method along with our fully discrete approximation $X_{h,\Delta t}^T$ of $X(T)$, we must therefore generate many samples of $X_{h,\Delta t}^T$. In practice one samples the vector $\bar{x}_h^T = [x_1, x_2, \ldots, x_N]$, of coefficients of the expansion $X_{h,\Delta t}^T = \sum_{k=1}^{N_h} x_k \Phi_k^h$, where $\Phi^h = (\Phi_k^h)_{k=1}^{N_h}$ is a basis of $V_h$.

We consider two approaches, the first of which is the classical approach of path-based sampling, i.e., solving the $N_{\Delta t}$ matrix equations corresponding to the backward Euler system (3) once for each sample $i = 1, 2, \ldots, N$ (Algorithm 1). These systems are obtained by expanding (3) on $\Phi^h$ and applying $\langle \Phi^h_i, \cdot \rangle$ to each side of this equality for $i = 1, 2, \ldots, N_h$.

**Algorithm 1** Path-based Monte Carlo method of computing an estimate $E_N[\phi(X_{h,\Delta t}^T)]$ of $E[\phi(X(T))]$

1: result = 0
2: for $i = 1$ to $N$ do
3:    Sample a realization $W^{(i)}$ of the Q-Wiener process $W$
4:    Compute $\bar{x}_h^T = [x_1, x_2, \ldots, x_N]$ directly by solving the matrix equations corresponding to (3) driven by $W^{(i)}$
5:    Compute $\phi(X_{h,\Delta t}^T) = \phi \left( \sum_{k=1}^{N_h} x_k \Phi_k^h \right)$
6:    result = result + $\phi(X_{h,\Delta t}^T)^{(i)} / N$
7: end for
8: $E_N[\phi(X_{h,\Delta t}^T)] = result$

The second approach is that of covariance-based sampling where the covariance $\text{Cov}(X_{h,\Delta t})$ is computed, yielding the covariance matrix of $\bar{x}_{h,\Delta t}^T$ which can be used to generate samples of $\bar{x}_{h,\Delta t}^T$ directly (Algorithm 2). This is possible since $X_{h,\Delta t}^{j+1}$ of (3) is Gaussian, being a sum of a deterministic affine linear transformation of the $\mathcal{F}_t$-measurable Gaussian random variable $X_{h,\Delta t}^T$ and the Gaussian random variable $P_hG(t) \Delta W^j$ which is independent of $\mathcal{F}_t$.

In the next theorem we introduce the scheme we use for the calculation of $\text{Cov}(X_{h,\Delta t})$. It is inspired by a technique for the derivation of stability properties of SDE approximation schemes (cf. [5]). In order to avoid long formulas, we introduce the abbreviations $R_{h,\Delta t} = (I_H - \Delta t A_h)$, $F_{h,\Delta t}^{1,j} = \left( I_H + \Delta t P_h F_{t_j}^1 \right)$, and $F_{h,\Delta t}^{2,j} = \Delta t P_h F_{t_j}^2$, so that (3) can be written as

$$R_{h,\Delta t} X_{h,\Delta t}^{j+1} = F_{h,\Delta t}^{1,j} X_{h,\Delta t}^j + F_{h,\Delta t}^{2,j} + P_h G(t_j) \Delta W^j,$$

$$X_{h,\Delta t}^{j+1} = R_{h,\Delta t} X_{h,\Delta t}^j + F_{h,\Delta t}^{1,j} X_{h,\Delta t}^j + F_{h,\Delta t}^{2,j} + P_h G(t_j) \Delta W^j.$$
for \( j = 0, 1, \ldots, N_{\Delta t} - 1 \).

**Theorem 3.1.** Let the terms of (1) satisfy Assumption 2.1 and let \((X_{h,\Delta t}^j)_{j=0}^{N_{\Delta t}}\) be given by the backward Euler scheme (3). Then the mean \(\mu^T \in V_h\) and covariance \(\Sigma^T \in V_h^{\otimes 2}\) of \(X_{h,\Delta t}^T\) is given by the recursions

\[
R_{h,\Delta t} \mu_{j+1}^{t_j} = F_{h,\Delta t}^{1,j} \mu_{j}^{t_j} + F_{h,\Delta t}^{2,j}
\]

and

\[
(R_{h,\Delta t})^{\otimes 2} \Sigma_{j+1}^{t_j} = (F_{h,\Delta t}^{1,j})^{\otimes 2} \Sigma_{j}^{t_j} + \mathbb{E} \left( (P_h G(t_j) \Delta W^j)^{\otimes 2} \right)
\]

for \( j = 0, 1, \ldots, N_{\Delta t} - 1 \).

**Proof.** We first prove the result for \( F \) linear, so that \( F_t^2 = 0 \) for all \( t \in [0, T] \).

The recursion scheme (6) for the mean follows trivially by applying \( \mathbb{E}[\cdot] \) to both sides of (5), noting that the expectation commutes with affine operators and that \( \Delta W^j \) has zero mean.

For the covariance recursion scheme (7), we first tensorize (5) to get

\[
(R_{h,\Delta t})^{\otimes 2} \left( X_{h,\Delta t}^{t_{j+1}} \right) = (F_{h,\Delta t}^{1,j})^{\otimes 2} \left( X_{h,\Delta t}^{t_j} \right) + (P_h G(t_j) \Delta W^j) \otimes (P_h G(t_j) \Delta W^j)
\]

By using the independence of \( \Delta W^j \) and \( X_{h,\Delta t}^{t_j} \), along with the zero mean property of the former term, we get

\[
\mathbb{E} \left[ F_{h,\Delta t}^{1,j} X_{h,\Delta t}^{t_j} \otimes P_h G(t_j) \Delta W^j \right] = \mathbb{E} \left[ F_{h,\Delta t}^{1,j} X_{h,\Delta t}^{t_j} \right] \otimes \mathbb{E} [P_h G(t_j) \Delta W^j] = 0
\]

and similarly, the mean of the third term of (8) is also zero. Putting this together, we obtain that the mean of (8) is given by

\[
(R_{h,\Delta t})^{\otimes 2} \mathbb{E} \left[ X_{h,\Delta t}^{t_{j+1}} \right] = (F_{h,\Delta t}^{1,j})^{\otimes 2} \mathbb{E} \left[ X_{h,\Delta t}^{t_j} \right] + \mathbb{E} \left[ (P_h G(t_j) \Delta W^j)^{\otimes 2} \right].
\]

Tensorizing (6), the recursion scheme for the mean, we get

\[
(R_{h,\Delta t})^{\otimes 2} \left( \mu_{j+1}^{t_j} \right) = (F_{h,\Delta t}^{1,j})^{\otimes 2} \left( \mu_{j}^{t_j} \right)
\]

and by subtracting this from the previous equation we end up with (7). The general case of a non-zero \( F_{h,\Delta t}^{2,j} \) term is proven in the same way, noting that all terms involving this disappears from (7) when subtracting the tensorized mean in the last step. \( \Box \)

**Remark 3.2.** Note that the computation of the covariance above can easily be extended to the case of multiplicative noise, i.e., when \( G \) depends linearly on \( X \). However, the approximation is then no longer Gaussian, so we cannot use the covariance for sampling.

Next, we compare the computational complexities of Algorithms 1 and 2. In order to do this, we first need to know how to optimally choose the sample size \( N \) with respect to the discretization parameters \( h \) and \( \Delta t \). Combining (4) with Theorem 2.5 we get, using the triangle inequality, for a constant \( C > 0 \),

\[
\| \mathbb{E}[\phi(X(T))] - E_N[\phi(X_{h,\Delta t}^T)] \|_{L^2(\Omega; \mathbb{R})} \leq \| \mathbb{E}[\phi(X(T))] - \mathbb{E}[\phi(X_{h,\Delta t}^T)] \|_{L^2(\Omega; \mathbb{R})} + \| E_N[\phi(X_{h,\Delta t}^T)] - E_N[\phi(X_{h,\Delta t}^T)] \|_{L^2(\Omega; \mathbb{R})}
\]
Algorithm 2 Covariance-based Monte Carlo method of computing an estimate \( E_N[\phi(X_{h,\Delta t}^T)] \) of \( E[\phi(X(T))] \)

1: Form the mean vector \( \mu \) and covariance matrix \( \Sigma \) of \( \bar{x}_h^T \) by solving the matrix equations corresponding to (6) and (7)
2: \( \text{result} = 0 \)
3: for \( i = 1 \) to \( N \) do
4: \( \text{Sample } \bar{x}_h^T = [x_1, x_2, \ldots, x_{N_h}]^T \sim N(\mu, \Sigma) \)
5: \( \text{Compute } \phi(X_{h,\Delta t}^T) = \phi \left( \sum_{k=1}^{N_h} x_k \Phi_k^h \right) \)
6: \( \text{result} = \text{result} + \phi(X_{h,\Delta t}^T)^{(i)}/N \)
7: end for
8: \( E_N \left[ \phi(X_{h,\Delta t}^T) \right] = \text{result} \)

\[
\leq C \left( (1 + |\log(h)|) \left( h^2 + \Delta t^\delta \right) + N^{-1/2} \right).
\]

To balance this error we choose \( \Delta t \) and \( N \) so that \( \Delta t^\delta \simeq N^{-1/2} \simeq h^2 \). Given this, we make the following assumption (cf. [3, 4]) in order to compute bounds on the computational complexities of Algorithm 1 and 2.

**Assumption 3.3.** There is a \( d \in \mathbb{N} \) such that the cost of solving (3) once to get \( X_{h,\Delta t}^{T+j} \) given \( X_{h,\Delta t}^T \) for \( j = 0, \ldots, N_{\Delta t} - 1 \) is \( O(h^{-d}) \) while the cost of solving the corresponding tensorized system (7) once is \( O(h^{-2d}) \). Furthermore, the cost of computing a sample of a Gaussian \( V_h \)-valued random variable with a covariance given by (7) is assumed to be \( O(h^{-2d}) \).

**Remark 3.4.** In our model problem Example 2.2, \( d \) is the dimension of the space \( \mathbb{R}^d \) in which the domain \( D \) is contained and the dimension of \( V_h \) is typically \( O(h^{-d}) \).

In order to compute an approximation of \( E(\phi(X(T))) \), if we use Algorithm 1, we need to solve the backward Euler system (3) \( N \cdot N_{\Delta t} = N\Delta t^{-1} \) times, making the total cost \( O(N\Delta t^{-1}h^{-d}) = O(h^{-4-d-2/\delta}) \). If we use Algorithm 2 instead, we need to solve (7) \( N_{\Delta t} = \Delta t^{-1} \) times and then sample from the resulting covariance \( N \) times, making the total cost \( O(h^{-2d-2/\delta}) + O(h^{-2d-4}) \). We collect these observations in the following proposition, which ends this section.

**Proposition 3.5.** Let \( \phi \) and the terms of (1) satisfy Assumptions 2.1 and 2.4. Assume that \( X_{h,\Delta t}^T \) is given by the recursion (3) and that \( X(T) \) is the solution to (1) at time \( T < \infty \). If \( N \simeq h^{-4} \) and \( \Delta t \simeq h^{2/\delta} \) then there is a constant \( C > 0 \), not depending on \( h \), such that

\[
\| E(\phi(X(T))) - E_N[\phi(X_{h,\Delta t}^T)] \|_{L^2(\Omega; \mathbb{R})} \leq C \left( 1 + |\log(h)| \right) h^2.
\]

Under Assumption 3.3, the cost of computing \( E_N[X_{h,\Delta t}^T] \) with Algorithm 1 is bounded by \( O(h^{-4-d-2/\delta}) \) while the cost of computing it with Algorithm 2 is bounded by \( O(h^{-2d-2/\delta}) + O(h^{-2d-4}) \).

4. Covariance-based sampling in a multilevel Monte Carlo setting

For our goal of efficiently estimating \( E(\phi(X(T))) \), the multilevel Monte Carlo algorithm can be a more efficient alternative to the standard Monte Carlo algorithm. For a sequence \( (Y_\ell)_{\ell \in \mathbb{N}_0} \)
of random variables in \( L^2(\Omega; \mathbb{R}) \) approximating \( Y \in L^2(\Omega; \mathbb{R}) \), where the index \( \ell \in \mathbb{N}_0 \) is referred to as a level, we recall that the multilevel Monte Carlo estimator \( E^{L} \) of \( Y_L \in (Y_\ell)_{\ell \in \mathbb{N}_0} \) is, for \( L \in \mathbb{N} \), defined by

\[
E^{L}[Y_L] = E_{N_0}[Y_0] + \sum_{\ell=1}^{L} E_{N_\ell}[Y_\ell - Y_{\ell-1}],
\]

where \((N_\ell)_{\ell=0}^L\) consists of level specific numbers of samples in the respective Monte Carlo estimators.

To apply this algorithm in our setting, we take a sequence \((X^T_\ell)_{\ell \in \mathbb{N}_0}\) of approximations of \( X(T) \), given by \( X^T_\ell = X^T_{h_\ell, \Delta t_\ell} \), where \((h_\ell)_{\ell \in \mathbb{N}_0}\) is a decreasing sequence of mesh sizes and \( \Delta t_\ell \approx h_\ell^2 \) so that \((\phi(X^T_\ell))_{\ell \in \mathbb{N}_0}\) becomes a sequence approximating \( \phi(X(T)) \). We set \( X^T_1 = 0 \). Computing \( E^{L} [\phi(X^T_\ell)] \) involves, for each \( \ell = 1, 2, \ldots, L \), sampling \( \phi(X^T_\ell) - \phi(X^T_{\ell-1}) \) \( N_\ell \) times (we specify how to choose the sample sizes below). For this it is key that \( X^T_\ell \) on the fine level \( \ell \) and \( X^T_{\ell-1} \) on the coarse level \( \ell - 1 \) are positively correlated. In the classical path-based method (Algorithm 3, see also [1, 3, 4, 12]), this is achieved by computing them using the same realization of the driving \( Q \)-Wiener process.

**Algorithm 3**: Path-based multilevel Monte Carlo method of computing an estimate \( E^{L} [\phi(X^T_\ell)] \) of \( E[\phi(X(T))] \)

1: \( \text{result} = 0 \)
2: for \( \ell = 0 \) to \( L \) do
3: for \( i = 1 \) to \( N_\ell \) do
4: Sample a realization \( W^{(i)} \) of the \( Q \)-Wiener process \( W \)
5: Compute \( \bar{x}^T_{h_{\ell-1}} = [x^T_{1,1}, x^T_{2,1}, \ldots, x^T_{N_{h_{\ell-1}},1}]' \) by solving the matrix equations corresponding to (3) driven by \( W^{(i)} \)
6: Compute \( \bar{x}^T_{h_\ell} = [x^T_{1,1}, x^T_{2,1}, \ldots, x^T_{N_{h_\ell},1}]' \) by solving the matrix equations corresponding to (3) driven by \( W^{(i)} \)
7: Compute \( \phi(X^T_\ell) - \phi(X^T_{\ell-1}) = \phi \left( \sum_{k=1}^{N_{h_\ell}} x^T_{k,1} \Phi_{k}^{h_\ell} \right) - \phi \left( \sum_{k=1}^{N_{h_{\ell-1}}} x^T_{k,1} \Phi_{k}^{h_{\ell-1}} \right) \)
8: result = result + (\( \phi(X^T_\ell) - \phi(X^T_{\ell-1}) \)) / \( N_\ell \)
9: end for
10: end for
11: \( E^{L} [\phi(X^T_\ell)] = \text{result} \)

In order to better understand the covariance-based method we introduce, we rewrite the approach of the path-based method as a system on the space \( V_{h'} \oplus V_h \). Consider to this end, for \( h, h', \Delta t, \Delta t' > 0 \), a pair \( (X^{t_j}_{h', \Delta t'})_{j=0}^{N_{\Delta t'}}, (X^{t_j}_{h, \Delta t})_{j=0}^{N_{\Delta t}} \) of approximations of \( X \), given by the backward Euler scheme (3). Assume further that they are nested in time, i.e., that \( \Delta t' = K \Delta t \) for some \( K \in \mathbb{N} \) with \( K > 1 \). Then we can create an extension \( (X^{t_j}_{h', \Delta t'})_{j=0}^{N_{\Delta t'}} \) of the coarse approximation \( (X^{t_j}_{h', \Delta t'})_{j=0}^{N_{\Delta t'}} \) to the finer time grid by the scheme

\[
\hat{F}_{h', \Delta t'}^{1,j} X^{t_{j+1}}_{h', \Delta t'} = \hat{F}_{h', \Delta t'}^{1,j} X^{t_j}_{h', \Delta t'} + \hat{F}_{h', \Delta t'}^{2,j} + P_{h'} \hat{G}(t_j) \Delta W^j,
\]
for \( j = 0, 1, \ldots, N_{\Delta t} - 1 \), where \( \Delta W^j = W(t_{j+1}) - W(t_j) \). The operators are given by

\[
\tilde{R}_{j}^* \Delta t' = \begin{cases} 
\tilde{R}_{j}^* \Delta t' & \text{if } j + 1 = 0 \mod K, \\
I_H & \text{otherwise},
\end{cases}
\]

\[
\tilde{F}_{j}^* \Delta t' = \begin{cases} 
\tilde{F}_{j}^* \Delta t' / K & \text{if } j + 1 = 1 \mod K, \\
0 & \text{otherwise},
\end{cases}
\]

Note that \( \tilde{X}_{j+1}^* = X_{j+1}^* / K \) when \( j + 1 = 0 \mod K \) since then

\[
\tilde{R}_{j}^* \Delta t' \tilde{X}_{j+1}^* = \tilde{F}_{j}^* \Delta t' \tilde{X}_{j}^* + \tilde{F}_{j}^* \Delta t' + P_h \tilde{G}(t_j) \Delta W^j = \tilde{X}_{j}^* + P_h \tilde{G}(t_j) \Delta W^j = \cdots
\]

where \( \Delta W^j = W(t_{j+1}) - W(t_j) \). Hence, the scheme is equivalent to solving the system

\[
\begin{bmatrix}
\tilde{R}_{j}^* \Delta t' & 0 \\
0 & \tilde{R}_{j}^* \Delta t'
\end{bmatrix}
\begin{bmatrix}
\tilde{X}_{j+1}^* \\
\tilde{X}_{j}^*
\end{bmatrix}
= \begin{bmatrix}
\tilde{F}_{j}^* \Delta t' & 0 \\
0 & \tilde{F}_{j}^* \Delta t'
\end{bmatrix}
\begin{bmatrix}
\tilde{X}_{j+1}^* \\
\tilde{X}_{j}^*
\end{bmatrix} + \begin{bmatrix}
\tilde{F}_{j}^* \Delta t' \\
\tilde{F}_{j}^* \Delta t'
\end{bmatrix} + \begin{bmatrix}
P_h \tilde{G}(t_j)
\end{bmatrix} \Delta W^j
\]

in \( V_h' \oplus V_h \) for \( j = 0, 1, \ldots, N_{\Delta t} - 1 \). We note that \( \tilde{X}_{j+1}^* \Delta t' \) is a Gaussian \( V_h' \oplus V_h \)-valued random variable for all \( j = 0, 1, \ldots, N_{\Delta t} - 1 \). Therefore, a covariance-based approach to sampling \( (\tilde{X}_{j}^* \Delta t', \tilde{X}_{j}^* \Delta t') \) can be obtained by directly computing \( \text{Cov}(X_{j}^* \Delta t', X_{j}^* \Delta t') = \text{Cov}(\tilde{X}_{j}^* \Delta t', \tilde{X}_{j}^* \Delta t') \). However, to save on computational power, we base Algorithm 4 on computing the cross-covariance \( \text{Cov}(X_{j}^* \Delta t', X_{j}^* \Delta t) \) instead. The scheme for this quantity is formulated in the next theorem.

**Theorem 4.1.** Let the terms of (1) satisfy Assumption 2.1 and let, for \( h, h', \Delta t, \Delta t' > 0 \), \( (X_{j}^* \Delta t')_{j=0}^{N_{\Delta t}} \) and \( (X_{j}^* \Delta t')_{j=0}^{N_{\Delta t}} \) be given by the backward Euler scheme (3). Assume further that \( \Delta t' = K \Delta t \) for some \( K \in \mathbb{N} \) with \( K > 1 \). Then the co-covariance \( \text{Cov}(X_{j}^* \Delta t', X_{j}^* \Delta t) \) is given by \( \Sigma_t \in V_h' \oplus V_h \), where the sequence \( \{(\Sigma_t)_{j=0}^{N_{\Delta t}} \} \) fulfills

\[
(\tilde{R}_{j}^* \Delta t' \otimes R_{h, \Delta t}) \Sigma_{j+1} = (\tilde{F}_{j}^* \Delta t' \otimes F_{h, \Delta t}) \Sigma_t + E \left[ P_h \tilde{G}(t_j) \Delta W^j \otimes P_h G(t_j) \Delta W^j \right].
\]

**Proof.** The result is shown by deriving the scheme for \( \Sigma_t \) as \( \text{Cov}(\tilde{X}_{j}^* \Delta t, \tilde{X}_{j}^* \Delta t) = \mathbb{E}[(\tilde{X}_{j}^* \Delta t - E[\tilde{X}_{j}^* \Delta t]) \otimes (\tilde{X}_{j}^* \Delta t - E[\tilde{X}_{j}^* \Delta t])] \) in the same way as in Theorem 3.1, noting that for each \( j = 0, 1, \ldots, N_{\Delta t} - 1 \), both \( \tilde{X}_{j+1}^* \) and \( X_{j}^* \Delta t \) are the sum of an \( F_{j}^* \)-measurable and an \( F_{j}^* \)-independent random variable.

The following proposition, which is an adaption of [11, Theorem 1] to our setting, shows how one should choose the sample sizes in a multilevel Monte Carlo algorithm and provides bounds on the overall computational work for Algorithm 3 and 4.
Let \( h \) and \( \phi \) be differentiable mappings (cf. [10, Chapter 1] and [15, Example 4.2]) shows that there exists a constant \( C > 0 \) such that

\[
\| \phi'(X) \|_{L^2(\Omega, \mathbb{R})}^2 \leq C \| X - X(T) \|_{L^p(\Omega, H)}^2.
\]

**Algorithm 4** Covariance-based multilevel Monte Carlo method of computing an estimate \( E^L[\phi(X_T^\ell)] \) of \( E[\phi(X(T))] \)

1: \( \text{result} = 0 \)
2: for \( \ell = 0 \) to \( L \) do
3: \( \text{Compute the covariance matrix } \Sigma \) and mean vector \( \mu \) of
4: \( \hat{\mathbf{x}}_\ell = \left[ [\hat{\mathbf{x}}_{h_{\ell-1}}^T], [\hat{\mathbf{x}}_{h_{\ell}}^T] \right]' = \left[ x_{1}^{\ell-1}, x_{2}^{\ell-1}, \ldots, x_{N_{h_{\ell-1}}}^{\ell-1}, x_{1}^{\ell}, x_{2}^{\ell}, \ldots, x_{N_{h_{\ell}}}^{\ell} \right]' \)
5: \( \) by computing the means, covariances and cross-covariances of the pair \( (X_{\ell-1}^T, X_\ell^T) \) via the solution of the matrix equations corresponding to (6), (7) and (9)
6: for \( i = 1 \) to \( N_\ell \) do
7: \( \) \( \text{Sample } \hat{\mathbf{x}}_\ell \sim N(\mu, \Sigma) \)
8: \( \) \( \text{Compute } \phi(X_\ell^T) - \phi(X_{\ell-1}^T) = \phi \left( \sum_{k=1}^{N_{h_\ell}} x_k^\ell \Phi_k^\ell \right) - \phi \left( \sum_{k=1}^{N_{h_{\ell-1}}} x_k^{\ell-1} \Phi_k^{\ell-1} \right) \)
9: \( \) \( \text{result} = \text{result} + (\phi(X_\ell^T) - \phi(X_{\ell-1}^T))/N_\ell \)
10: \( \text{end for} \)
11: \( \text{end for} \)
12: \( E^L[\phi(X_T^\ell)] = \text{result} \)

**Proposition 4.2.** Let \( \phi \) and the terms of (1) satisfy Assumptions 2.1 and 2.4. Let \( (h_\ell)_{\ell \in \mathbb{N}_0} \) be a sequence of maximal mesh sizes that satisfy \( h_\ell \simeq a^{-\ell} \) for some \( a \in \mathbb{R} \) and all \( \ell \in \mathbb{N}_0 \). Let \( (X_\ell^T)_{\ell \in \mathbb{N}_0} \) be a sequence of approximations of \( X(T) \), where \( X_\ell^T = X_{\ell, \Delta t_{\ell}}^T \) is given by the recursion (3) with \( \Delta t_{\ell} \simeq h_\ell^2 \).

For \( L \in \mathbb{N}, \ell = 1, \ldots, L, \epsilon > 0 \), set \( N_\ell = [h_L^{-4}h_{\ell}^{2+\epsilon}] \), where \([\cdot]\) is the ceiling function, and \( N_0 = [h_L^{-4}] \). Then there exists a constant \( C > 0 \), dependent on \( a \) and \( \epsilon \) but not on \( L \), such that

\[
\| E[\phi(X(T))] - E^L[\phi(X_T^\ell)] \|_{L^2(\Omega, \mathbb{R})} \leq C(1 + |\log(h_L)|)h_L^2.
\]

**Proof.** By [11, Lemma 2] we have

\[
\| E[\phi(X(T))] - E^L[\phi(X_T^\ell)] \|_{L^2(\Omega, \mathbb{R})} \leq \| E[\phi(X(T)) - \phi(X_T^\ell)] \|_{L^2(\Omega, \mathbb{R})} + \sum_{\ell=1}^{L} N_{\ell-1}^{-1} \| \phi(X_\ell^T) - \phi(X_{\ell-1}^T) \|_{L^2(\Omega, \mathbb{R})}^2 \right)^{1/2}
\]

By the fact that the Fréchet derivative \( \phi' \) is at most polynomially growing and the uniform bound on the fully discrete solution of Theorem 2.3, there is a constant \( C > 0 \) such that

\[
\| \phi'(X_0^T) \|_{L^2(\Omega, \mathbb{R})}^2 < C.
\]

Furthermore, an application of the mean-value theorem for Fréchet differentiable mappings (cf. [10, Chapter 1] and [15, Example 4.2]) shows that there exists \( p \geq 2 \), independent of \( \ell \), such that

\[
\| \phi(X_\ell^T) - \phi(X(T)) \|_{L^2(\Omega, \mathbb{R})}^2 \leq C \| X_\ell^T - X(T) \|_{L^p(\Omega, H)}^2.
\]
Hence, using Theorem 2.3, we get that for a constant $C > 0$,
\[
\| \phi(X^T_\ell) - \phi(X^T_{\ell-1}) \|_{L^2(\Omega, \mathbb{R})}^2 \leq C \left( \| X^T_\ell - X(T) \|_{L^p(\Omega; H)}^2 + \| X^T_{\ell-1} - X(T) \|_{L^p(\Omega; H)}^2 \right)
\]
\[
\leq C(h^2_\ell + h^2_{\ell-1}) \leq C(1 + a^2)h^2_\ell.
\]
Using this along with Theorem 2.5 in (10) yields the existence of a constant $C$ such that
\[
\| \mathbb{E}[\phi(X(T))] - E^L[\phi(X^T_\ell)] \|_{L^2(\Omega, \mathbb{R})} \leq C \left( (1 + |\log(h_L)|)h^2_L + \left( N_0^{-1} + \sum_{\ell=1}^L N_{\ell-1}^{-1} h^2_\ell \right)^{1/2} \right)
\]
\[
\leq C h^2_L \left( 1 + |\log(h_L)| + (1 + \zeta(1+\epsilon))^{1/2} \right),
\]
where $\zeta$ denotes the Riemann zeta function and the last inequality follows from the choice of sample sizes. This shows the first part of the theorem.

If we use Algorithm 3 to compute $E^L[\phi(X^T_0)]$, the cost of sampling $X^T_0$ $N_0$ times is by Proposition 3.5 $O(N_0 h_0^{-d-2/\delta}) = O(h^{-4}_0)$. Similarly, since the computation of $\phi(X^T_\ell) - \phi(X^T_{\ell-1})$, $1 \leq \ell \leq L$, is dominated by the sampling of $X^T_\ell$, the cost for the rest of the terms is bounded by a constant times
\[
\sum_{\ell=1}^L N_\ell h^{-d-2/\delta}_\ell = \sum_{\ell=1}^L h^{-4}_L h^{2-d-2/\delta}_\ell \ell^{1+\epsilon} \leq h^{-2d-2/\delta}_L L^{2+\epsilon}.
\]
For Algorithm 4, the cost of sampling $X^T_0$ $N_0$ times is still $O(h^{-4}_0)$. For $1 \leq \ell \leq L$, the cost of computing the covariance of $X^T_\ell$, $X^T_{\ell-1}$ and their cross-covariance is dominated by the cost of computing the covariance of $X^T_\ell$, which is, by the same reasoning as that which precedes Proposition 3.5, $O(h^{-2d-2/\delta}_\ell)$. The cost of sampling a positively correlated pair of $X^T_\ell$ and $X^T_{\ell-1}$, given that all covariances have been computed, is $O(h^{-2d}_\ell) + O(h^{-2d}_{\ell-1}) = O(h^{-2d}_\ell)$ so the total cost for sampling $\phi(X^T_\ell) - \phi(X^T_{\ell-1})$ for all $\ell = 1, 2, \ldots, L$ is bounded by a constant times
\[
\sum_{\ell=1}^L \left( h^{-2d-2/\delta}_\ell + N_\ell h^{-2d}_\ell \right) = \sum_{\ell=1}^L \left( h^{-2d-2/\delta}_\ell + h^{-4}_L h^{2-2d}_\ell \ell^{1+\epsilon} \right)
\]
\[
\leq 2 \max(h^{-2d-2/\delta}_L, h^{-2d-2d}_L L^{1+\epsilon}).
\]

Hence, in the case of $\delta = 1/2$, covariance-based sampling combined with classical Monte Carlo appears to be the best method for $d = 1, 2$. For $\delta = 1$, on the other hand, covariance-based sampling combined with MLMC should be used for $d = 1, 2$. For $d = 3$ the classical path-based MLMC it the optimal algorithm.

Let us conclude this section with the remark that in the absence of weak rates, strong rates can still be used to choose the sample sizes in the standard and the multilevel Monte Carlo estimators provided that $\phi$ fulfill a Lipschitz condition. However, the resulting tuning can be suboptimal, cf. [11]. Furthermore, there exists results on weak convergence for similar schemes to the one considered in [10] with different assumptions on the parameters of (1) and on $\phi$, for example [2]. If these are used to tune the Monte Carlo estimators, the conclusions regarding which methods are best may be different.
5. Numerical simulations

In this section we continue with the setting of Example 2.2 and demonstrate our results numerically for the stochastic heat equation driven by additive (i.e., \( G = I \)) Wiener noise

\[ \text{d}X(t) = \Delta X(t) \text{d}t + dW(t), \]

on \( H = L^2(D) \) with \( D = (0,1) \), for \( t \in (0,T) = (0,1] \) with deterministic initial value \( X(0) = x_0 = \sin(2\pi \cdot) \) and Dirichlet zero boundary conditions. The covariance function of \( W \) is for \( x,y \in D \) chosen to be \( q(x,y) = 20 \exp(-2|x-y|) \). For the spatial discretization of (11), take \((T_h)_{h \in (0,1]}\) to be a family of uniform triangulations of (0,1) with \( h \) being the mesh size. Let \( V_h \) be the space of all functions that are continuous and piecewise linear on \( T_h \) and zero at the boundary of \((0,1)\). For a given \( h > 0 \), we denote by \( \Phi^h = (\Phi^h)_{i=1}^{N_h} \) the standard basis of \( \hat{V} \) and zero at the boundary of \((0,1)\). Below we compute approximations of \( \mathbb{E}[\phi(X(T))] \), with \( \phi(\cdot) = \| \cdot \|^2 \in C^2_p(H;\mathbb{R}) \) using Algorithms 1-4. We briefly describe the matrix forms of the problems which we use for the simulation.

We recall that the system of equations in \( \mathbb{R}^{N_h} \) corresponding to (3) is given by

\[ (M_h - \Delta(t A_h)) x_h^{j+1} = M_h x_h^j + \Delta W_h^j \]

for \( j = 0,1,\ldots,N_{\Delta t} - 1 \) to get the vector \( x_h^T \). Here \( M_h \) is the mass matrix, \(-A_h \) the stiffness matrix and \( (\Delta W_h^j)_{j=0}^{N_{\Delta t} - 1} \) a family of iid (independent and identically distributed) Gaussian \( \mathbb{R}^{N_h} \)-valued random vectors with covariance matrix \( \Sigma_{h,\Delta W} \), the entries \((s_{i,j})_{i,j \in \{1,2,\ldots,N_h\}}\) of which are given by

\[ s_{i,j} = \Delta t \int_{D^2} q(x,y) \Phi^h_i(x) \Phi^h_j(y) \, dx \, dy \]

for row \( i \) and column \( j \in \{1,2,\ldots,N_h\} \).

We get a system of equations in \( \mathbb{R}^{2N_h} \) for the covariance recursion scheme of Theorem 3.1 by expanding (7) and applying \( \left( \Phi^2_h \right) \) to each side of this equality for \( i = 1,2,\ldots,N_h^2 \), where \( \Phi^2_h = (\Phi^2_h)_{i=1}^{N_h^2} \) is a basis of \( \hat{V} \). Here it is key that we choose \( \Phi^2_h = \Phi^h \left( \frac{(i-1)}{N_h} \right) + \ldots + \Phi^h \left( \frac{(i-1)}{N_h} \right) \) for \( i = 1,2,\ldots,N_h^2 \) since then the matrices corresponding to \( (R_{h,\Delta t}) \) and \( (F_{h,\Delta t}) \) will simply be Kronecker products of the matrices corresponding to \( (R_{h,\Delta t}) \) and \( (F_{h,\Delta t}) \), \( j = 0,1,\ldots,N_{\Delta t} - 1 \). As for the vector corresponding to the covariance of the Wiener increment, we have, using the properties of the covariance operator as noted in Section 2,

\[
\begin{align*}
\left( \mathbb{E}[\Delta W \otimes \Delta W], \Phi^h \left( \frac{(i-1)}{N_h} \right) + \ldots + \Phi^h \left( \frac{(i-1)}{N_h} \right) \right)_{H \otimes H} \\
= \mathbb{E} \left[ \left( \Delta W, \Phi^h \left( \frac{(i-1)}{N_h} \right) + \ldots + \Phi^h \left( \frac{(i-1)}{N_h} \right) \right) \right] \\
= \Delta t \int_{D^2} q(x,y) \Phi^h \left( \frac{(i-1)}{N_h} \right) \, dx \, dy,
\end{align*}
\]

which means that this vector is simply the vectorization of the symmetric matrix \( \Sigma_{h,\Delta W} \). The system of equations for the covariance in \( \mathbb{R}^{2N_h} \) is therefore given by

\[ (M_h - \Delta(t A_h))_{\otimes \otimes} \Sigma_{h,\Delta W}^{\otimes \otimes} = M_h_{\otimes \otimes} \Sigma_{h,\Delta W}^{\otimes \otimes} + \text{Vec} \left( \Sigma_{h,\Delta W} \right) \]
for \( j = 0, 1, \ldots, N_\Delta - 1 \), where \( \otimes_K \) denotes the Kronecker product and \( \text{Vec} \) the vectorization operator. In other words, for this choice of basis, \( \mathbf{y}_h^T \) is simply the vectorization of the covariance matrix \( \Sigma_{\mathbf{S}_h^T} \), the end result of (12). The sampling of \( \mathbf{x}_h^T \) is accomplished by means of a Cholesky decomposition of this matrix.

In Figure 1(a) we show, for both the path- and covariance-based methods, estimates

\[
\left( \sum_{i=1}^{5} \left( \mathbb{E}[\phi(X(T))] - E_N[\phi(X_{h,\Delta_t}^T)](i) \right)^2 \right)^{1/2},
\]

for 5 different realizations of \( E_N[\phi(X_{h,\Delta_t}^T)] \), of the mean squared errors

\[
\| \mathbb{E}[\phi(X(T))] - E_N[\phi(X_{h,\Delta_t}^T)] \|_{L^2(\Omega; \mathbb{R})}
\]

for \( h = 2^{-1}, 2^{-2}, \ldots, 2^{-5} \), with \( \Delta t \) and \( N \) chosen according to Proposition 3.5. In the case of the covariance-based method, we also include \( h = 2^{-6} \). The quantity \( \mathbb{E}[\phi(X(T))] \) is replaced by a reference solution \( \mathbb{E}[\phi(X_{h,\Delta_t}^T)] \), with \( h = 2^{-8} \), computed with a deterministic method, cf. [15, Section 6]. As expected, the order of convergence is \( O(h^2) \). In Figure 1(b) we show the computational cost in seconds along with the corresponding upper bounds on the costs from Proposition 3.5. The costs for the path-based method appear to roughly follow the bounds while the covariance-based appear to perform better than its complexity bound. The reason for this is that we have assumed that the cost of sampling is quadratic with respect to \( N_h \). Since we use a triangular matrix for the sampling, the actual complexity is for small \( N_h \) more linear than quadratic.

\[
\begin{array}{c}
\text{Convergence, Monte Carlo} \\
\text{Path + MC} \quad \text{Cov + MC} \quad \text{O(h}^2) \\
\end{array}
\]

\[
\begin{array}{c}
\text{Computational cost, Monte Carlo} \\
\text{Path + MC} \quad \text{Cov + MC} \quad \text{O(h}^{-6}) \\
\end{array}
\]

(a) Mean square errors of the MC estimator for the path- and covariance-based methods of Proposition 3.5. (b) Computational costs in seconds for the simulations of Figure 1(a) with bounds from Proposition 3.5.

Figure 1. Convergence and computational costs of the singlelevel Monte Carlo estimator (Algorithms 1 and 2).

For the multilevel Monte Carlo estimator \( \mathbb{E}[\phi(X_L^T)] \) we set, for \( \ell = 0, \ldots, L, h_\ell = 2^{-\ell-1} \) and choose the temporal step sizes and sample sizes according to Proposition 4.2. At each level \( \ell = 1, 2, \ldots, L \), in order to compute \( \phi(X_\ell^T) - \phi(X_{\ell-1}^T) \) we must sample a positively
correlated pair \((X^T_i, X^T_{i-1})\). For details on how this is done in the path-based method (i.e., Algorithm 3) we refer to \cite{4}. For the covariance-based method of Algorithm 4, we first choose a basis \(\Phi^\ell = (\Phi^\ell_i)_{i=1}^{N_h \times N_h - 1}\) of \(V_{h_{\ell-1}} \otimes V_{h_{\ell}}\) by \(\Phi^\ell_i = \Phi_{h_{\ell-1}}^{(i-1)N_h} \otimes \Phi_{h_{\ell}}^{(i-1)N_h}\). Analogously to the derivation of \eqref{13}, this transforms \eqref{7} into a system of equations which yields the coefficients \(\vec{y}^T_\ell = [y_1^T, y_2^T, \ldots, y_{N_h \times N_h - 1}^T]^T\) of the cross-covariance \(\text{Cov}(X^T_{i-1}, X^T_i) = \sum_{i=1}^{N_h \times N_h - 1} y_i^T \Phi^h_{h_{\ell-1}}^{(i-1)N_h + 1} \otimes \Phi^h_{h_{\ell}}^{(i-1)N_h}N_h\). In the same way as before, \(\vec{y}^T_\ell\) can be seen to be the vectorization of the cross-covariance matrix \(\Sigma_{\vec{x}^T_{h_{\ell-1}} \vec{x}^T_{h_{\ell}}}\) of \(\vec{x}^T_{h_{\ell-1}}\) and \(\vec{x}^T_{h_{\ell}}\). Now, the vector \(\vec{x}^\ell = \left[\left[\vec{x}^T_{h_{\ell-1}}\right]', \left[\vec{x}^T_{h_{\ell}}\right]'\right]'\) has covariance matrix \(\Sigma_{\vec{x}^\ell}\) given by

\[
(14) \quad \Sigma_{\vec{x}^\ell} = \begin{bmatrix}
\Sigma_{\vec{x}^T_{h_{\ell-1}} \vec{x}^T_{h_{\ell}}} & \Sigma_{\vec{x}^T_{h_{\ell-1}} \vec{x}^T_{h_{\ell}}} \\
\Sigma_{\vec{x}^T_{h_{\ell-1}} \vec{x}^T_{h_{\ell}}} & \Sigma_{\vec{x}^T_{h_{\ell}}}
\end{bmatrix},
\]

where the diagonal entries are obtained via \eqref{13} as before. The sampling is again accomplished via a Cholesky decomposition of this matrix.

In Figure 2(a) we show the estimates

\[
\left(\sum_{i=1}^{5} \left( \mathbb{E}[\phi(X(T))] - E^L[\phi(X^T_i)^{(i)}] \right)^2 \right)^{1/2},
\]

for 5 different realizations of \(E^L[\phi(X^T_i)^{(i)}]\), of the mean squared errors

\[
||\mathbb{E}[\phi(X(T))] - E^L[\phi(X^T_i)]||_{L^2(\Omega; \mathbb{R})}
\]

for \(L = 0, 1, 2, \ldots, 5\). The quantity \(\mathbb{E}[\phi(X(T))]\) is again replaced with the reference solution from before. The order of convergence is again as expected. In Figure 2(b) we show the computational costs for these errors with the corresponding upper bounds on the costs from Proposition 4.2. We see a clear improvement in performance as compared to Figure 1(b), noting that the cost of the last computation for the covariance-based MLMC method is roughly half as big as the cost of the corresponding computation of the covariance-based MC method of Figure 1(b). Both methods appear to follow the derived complexity bounds.

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(a) Mean square errors of the MLMC estimator for the path- and covariance-based methods of Proposition 4.2.

(b) Computational costs in seconds for the simulations of Figure 2(a) with bounds from Proposition 4.2.

Figure 2. Convergence and computational costs of the multilevel Monte Carlo estimator (Algorithms 3 and 4).

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