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WIENER CHAOS VERSUS STOCHASTIC COLLOCATION METHODS FOR LINEAR ADVECTION-DIFFUSION-REACTION EQUATIONS WITH MULTIPLICATIVE WHITE NOISE*

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Abstract. We compare Wiener chaos and stochastic collocation methods for linear advection-reaction-diffusion equations with multiplicative white noise. Both methods are constructed based on a recursive multistage algorithm for long-time integration. We derive error estimates for both methods and compare their numerical performance. Numerical results confirm that the recursive multistage stochastic collocation method is of order Δ (time step size) in the second-order moments while the recursive multistage Wiener chaos method is of order $\Delta^{\mathsf{N}} + \Delta^2$ (N is the order of Wiener chaos) for advection-diffusion-reaction equations with commutative noises, in agreement with the theoretical error estimates. However, for noncommutative noises, both methods are of order one in the second-order moments.

Key words. Wong–Zakai approximation, spectral expansion, multistage, weak convergence

AMS subject classifications. Primary, 60H15; Secondary, 35R60, 60H40

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NOTATION.

q:	Number of Brownian motions (noises).
N:	Highest order of Hermite polynomial chaos.
n:	Number of basis modes in approximating the Brownian motion.
L:	Level of Smolyak sparse grid collocation.
M:	Number of Fourier collocation nodes in physical space.
Δ:	Element size (in time) for multielement spectral approximation of Brownian motion.
K:	Number of elements in time, which is T/Δ with T the final integration time.
δt:	Time step size for time discretization in the time interval $(0, \Delta]$.
$\eta(\mathsf{L}, \mathsf{n}q)$:	Number of sparse grid points at level L with dimension $\mathsf{n}q$.

1. Introduction. Partial differential equations (PDEs) driven by white noise have different interpretations of stochastic products and lead to different numerical approximations, unlike the PDEs driven by colored noise. Specifically, stochastic products for white noise are usually interpreted with two different products: the

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Ito product and the Stratonovich product; see e.g., [1]. Though a problem can be equivalently formulated using these two products, the use of different products leads to different performance of numerical solvers for PDEs driven by white noise, especially when Wiener chaos expansion (WCE) and stochastic collocation methods (SCM) in random space are used. In this paper, we will show theoretically and through numerical examples that for white noise driven PDEs, WCE and SCM have quite different performance when the noises are commutative. This is different from how WCE and SCM behave for PDEs driven by colored noise. For elliptic equations with colored noise, it is demonstrated in [3, 10] that there are only small differences in the numerical performance of generalized polynomial chaos expansion and SCM.

To apply WCE and SCM, we first discretize the Brownian motion with its truncated spectral expansion (see, e.g., [29, Chapter IX] and [21]), which results in PDEs with finite dimensional random inputs. Hence, our methods are Wong–Zakai type approximations [34, 35], where the Brownian motion is approximated by a smooth stochastic process of bounded variation, e.g., the spectral approximation used here and piecewise linear approximation of the Brownian motion [34, 35]. We note that piecewise linear approximation can be used instead, but this is beyond the scope of the paper.

The resulting PDEs can be solved numerically using a variety of space-time discretization methods and any sampling methods or functional expansion methods in random space. In random space, we will employ functional expansion methods, WCE [4, 21], and SCM [38], instead of the Monte Carlo method. These functional expansion methods have no statistical errors as no random number generators are used; they have only errors from truncations of Wiener processes and functional expansions and allow efficient short-time integration of stochastic PDEs (SPDEs) [4, 5, 15, 21, 22, 37, 38].

In principle, we can employ any functional expansion; however, different expansions are preferred for different stochastic products because of computational efficiency. In practice, WCE is associated with the Ito–Wick product (see (2.9)), as the product is defined with Wiener chaos modes yielding a weakly coupled system (lower-triangular system) of PDEs for linear equations. On the other hand, SCM is associated with the Stratonovich product (see (2.15)), yielding a decoupled system of PDEs. These different formulations lead to different numerical performance, as we demonstrate in section 4; in particular, WCE can be of second-order convergence in time, while SCM is only of first-order in time in the second-order moments for commutative noises. Further, when the noises serve as the advection coefficients, SCM can be more accurate than WCE when both methods are of first-order convergence as the SCM (Stratonovich formulation) can lead to smaller diffusion coefficients than those for WCE (Ito formulation).

However, a fundamental limitation of these expansion methods is the exponential growth of error with time and the increasing complexity as the number of random variables is increasing, generated by the discretization of the Brownian motion. To deal with this complexity, a recursive WCE method was proposed in [21] for the Zakai equation of nonlinear filtering with uncorrelated observations. More recently, a recursive multistage approach was developed to efficiently solve linear stochastic advection-diffusion-reaction equations using WCE [37] or SCM [38].

To deal with the complexity in random space, some preprocessing procedures have been proposed; see, e.g., [8, 31]. In these procedures, we are seeking the solution in the form $u(t,x;\omega) = \mathbb{E}[u(t,x;\cdot)] + \sum_{i=1}^{\infty} Y_i(t,\omega)u_i(t,x)$. Then by imposing the spatial orthogonality of $u_i(x,t)$ and $\partial_t u_j(t,x)$ $(i,j = 1,2,\ldots)$, we can obtain an equivalent system of SPDEs: a PDE for $\mathbb{E}[u(t,x;\cdot)]$, a system of equations for $Y_i(t,\omega)$, and a system of equations for $u_i(t,x)$. In many applications, this procedure is efficient, even with few terms of $Y_i(t,\omega)$ and $u_i(t,x)$, as it may take advantage of some intrinsic sparsity structures of the underlying problems. However, this procedure requires some numerical methods to obtain $Y_i(t,\omega)$, such as WCE (e.g., in [8]) and Monte Carlo methods (e.g., in [31]). When WCE or SCM is used, the complexity in random space is still high and thus the procedure is not efficient for problems driven by Brownian motion, where many modes $Y_i(t,\omega)$ and $u_i(t,x)$ are required. Though these procedures can be applied here, we limit ourselves to the issue of using the deterministic integration methods, without using these procedures.

Some numerical results of WCE for SPDEs have been presented in [37] for linear advection-diffusion-reaction equations and in [15] for nonlinear SPDEs including the stochastic Burgers equation and the Navier–Stokes equations. Numerical results for SCM have also been provided in [38] for linear stochastic advection-diffusion-reaction equations and the stochastic Burgers equation. Numerical results have demonstrated that WCE [37] and SCM [38] in conjunction with the recursive multistage approach are efficient for long-time integration of linear advection-diffusion-reaction equations.

The main aim of the current paper is the derivation of theoretical error estimates for both WCE and SCM methods and subsequent comparison of the numerical performance of the two methods for commutative and noncommutative noises. In addition, we will develop a recursive multistage SCM, different than in [38], using a spectral truncation of Brownian motion. Specifically, in this paper we will derive the error estimate of WCE for linear advection-diffusion-reaction equations with white noise in the advection velocity and that of SCM with white noise in the reaction rate. We note that the convergence rate of WCE is known only for linear advection-diffusion-reaction equations with white noise in the reaction rate, although the convergence of WCE for linear advection-diffusion-reaction equations has been studied for some time [20, 21, 22, 23].

The paper is organized as follows. In section 2, we review the WCE and SCM for linear parabolic SPDEs and develop a new recursive SCM using a spectral truncation of Brownian motion, following the same recursive procedure as WCE in [21, 37, 38]. In section 3 we present the error estimates for both methods for linear advection-diffusion-reaction equations, with the proofs presented in section 5. In section 4, we present numerical results of WCE and SCM for linear SPDEs with both commutative and noncommutative noises and verify the error estimates of WCE and SCM for commutative noises.

2. Review of Wiener chaos and stochastic collocation.

In this section, we briefly review WCE and SCM for the following linear SPDE in the Ito form:

$$du(t,x) = \mathcal{L}u(t,x)\,dt + \sum_{k=1}^{q}\mathcal{M}_k u(t,x)\,dw_k(t),\ (t,x)\in(0,T]\times\mathcal{D},$$
$$u(0,x) = u_0(x), \quad x\in\mathcal{D}, \tag{2.1}$$

where $(w(t),\mathcal{F}_t) = (\{w_k(t), 1\le k\le q\}, \mathcal{F}_t)$ is a system of one-dimensional independent standard Wiener processes defined on a complete probability space $(\Omega,\mathcal{F},P)$ and

$$\mathcal{L}u(t,x) = \sum_{i,j=1}^{d} a_{i,j}(x)\,D_iD_ju(t,x) + \sum_{i=1}^{d} b_i(x)D_iu(t,x) + c(x)\,u(t,x),$$
$$\mathcal{M}_k u(t,x) = \sum_{i=1}^{d}\sigma_{i,k}(x)D_iu(t,x) + \nu_k(x)\,u(t,x), \tag{2.2}$$

and D_i is the spatial derivative in the x_i-direction. We assume that the domain $\mathcal{D}$ in $\mathbb{R}^d$ is such that the periodic boundary conditions can be imposed or that $\mathcal{D} = \mathbb{R}^d$. In the former case, we will consider periodic boundary conditions and in the latter the Cauchy problem.

We assume that there exist a constant $\delta_{\mathcal{L}} > 0$ and a real number $C_{\mathcal{L}}$ such that for any $v \in H^1(\mathcal{D})$,

$$\langle \mathcal{L}v, v\rangle + \frac{1}{2}\sum_{k=1}^{q} \left\|\mathcal{M}_k v\right\|^2 + \delta_{\mathcal{L}}\left\|v\right\|_{H^1}^2 \le C_{\mathcal{L}}\left\|v\right\|^2, \tag{2.3}$$

where $\langle \cdot, \cdot\rangle$ is the duality between the Sobolev spaces $H^{-1}(\mathcal{D})$ and $H^1(\mathcal{D})$ associated with the inner product over $L^2(\mathcal{D})$ and $\left\|\cdot\right\|$ is the $L^2(\mathcal{D})$-norm. Specifically, we require that the coefficients of operators $\mathcal{L}$ and $\mathcal{M}$ in (2.2) are uniformly bounded and that

$$\sum_{i,j=1}^{d}\left(2a_{i,j}(x) - \sum_{k=1}^{q}\sigma_{i,k}(x)\sigma_{k,j}(x)\right) y_i y_j \ge 2\delta_{\mathcal{L}}\left|y\right|^2, \quad x, y \in \mathcal{D},$$

in addition to the Lipschitz continuity of $a_{i,j}(x)$. If $\mathbb{E}[\left\|u_0\right\|^2$ is bounded ($\mathbb{E}[\cdot]$ is the expectation with respect to P), these assumptions are sufficient for a unique square-integrable solution of (2.1)–(2.2); see e.g., [23, 25].

The problem (2.1)–(2.2) is said to have commutative noises if

$$\mathcal{M}_k\mathcal{M}_j = \mathcal{M}_j\mathcal{M}_k, \quad 1 \le k, j \le q, \tag{2.4}$$

and to have noncommutative noises otherwise. When $q = 1$, (2.4) is satisfied and thus this is a special case of commutative noises. When $\mathcal{M}_k$ are zeroth-order operators, ($\sigma_{i,k} = 0$), (2.4) is satisfied and the problem also has commutative noises. The definition is consistent with that of commutative and noncommutative noises for stochastic ordinary differential equations; see, e.g., [26]. In section 4, we test our algorithms on examples with both commutative and noncommutative noises.

Remark 2.1. The problem (2.1)–(2.2) can be regarded as an approximation of a problem driven by a cylindrical Wiener process. Consider a cylindrical Wiener process $W(t,x) = \sum_{k=1}^{\infty}\lambda_k w_k(t)e_k(x)$, where $\sum_{k=1}^{\infty}\lambda_k^2 < \infty$, $\{w_k(t)\}$ are independent Wiener processes, and $\{e_k(x)\}_{k=1}^{\infty}$ is a complete orthonormal basis (CONS) in $L^2(\mathcal{D})$; see e.g., [9, 30]. Thus, we can view (2.1)–(2.2) as approximations of SPDEs driven by this cylindrical Wiener process.

In both WCE and SCM, we discretize the Brownian motion using the following spectral representations (see, e.g., [21, 37]):

$$\lim_{\mathsf{n}\to\infty}\mathbb{E}[(w(t) - w^{(\mathsf{n})}(t))^2] = 0, \quad w^{(\mathsf{n})}(t) = \sum_{i=1}^{\mathsf{n}}\xi_i\int_0^t m_i(s)\,ds,\ t \in [0,T], \tag{2.5}$$

where ξ_i are mutually independent standard Gaussian random variables and $\{m_i\}_{i=1}^{\infty}$ is a CONS in $L^2([0,T])$. The expansion (2.5) is an extension of Fourier expansion of Brownian motion that is the Wiener construction [29, Chapter IX]; see also [17, 18].

2.1. WCE. The WCE solution to (2.1) is defined with the Cameron–Martin basis [6] in Wiener chaos space, using Fourier–Hermite series. The corresponding coefficients are obtained by solving the associated *propagator*, which is a *lower-triangular* linear system of deterministic parabolic equations determined by (2.1). Specifically, the solution to (2.1) can be represented as

$$u(t,x) = \sum_{\alpha\in\mathcal{J}_q} \frac{1}{\sqrt{\alpha!}}\varphi_\alpha(t,x;u_0)\xi_\alpha, \quad t\in(0,T], \tag{2.6}$$

where $\mathcal{J}_q$ is the set of multi-indices $\alpha = (\alpha_{k,l})_{k,l\geq 1}$ of finite length, i.e.,

$$\mathcal{J}_q = \left\{\alpha = (\alpha_{k,l},\ 1\leq k\leq q),\ l\geq 1,\quad \alpha_{k,l}\in\{0,1,2,\ldots\},\ |\alpha| := \sum_{k,l}\alpha_{k,l} < \infty\right\}.$$

The random variables ξ_α are Cameron–Martin orthonormal basis, defined as

$$\xi_\alpha := \prod_\alpha \left(\frac{H_{\alpha_{k,l}}(\xi_{k,l})}{\sqrt{\alpha_{k,l}!}}\right), \quad \alpha\in\mathcal{J}, \tag{2.7}$$

where $\xi_{k,l} = \int_0^T m_l(s)\,dw_k(s)$, and H_n is the nth Hermite polynomial:

$$H_n(x) = (-1)^n e^{x^2/2}\frac{d^n}{dx^n}e^{-x^2/2}. \tag{2.8}$$

Under our assumptions, the SPDE (2.1) can be written in the following form using the Ito–Wick product (see, e.g., [14, section 2.5] and [22]):

$$\begin{aligned} &du(t,x) = \mathcal{L}u(t,x)\,dt + \sum_{k=1}^q \mathcal{M}_k u(t,x)\diamond dw_k(t),\ (t,x)\in(0,T]\times\mathcal{D},\\ &u(0,x) = u_0(x),\quad x\in\mathcal{D}, \end{aligned} \tag{2.9}$$

where the Ito–Wick product "$\diamond$" is defined for the Cameron–Martin basis (2.7) such that $\xi_\alpha\diamond\xi_\beta = \sqrt{\frac{(\alpha+\beta)!}{\alpha!\beta!}}\xi_{\alpha+\beta}$. By (2.6) and the Cameron–Martin theorem [6], we obtain the coefficients $\varphi_\alpha(t,x;u_0) = \mathbb{E}[\sqrt{\alpha!}u(t,x)\xi_\alpha]$. Approximating w_k with $w_k^{(\mathsf{n})}$ in (2.5), we substitute the representation (2.6) into (2.9) and then we can readily check that the coefficients $\varphi_\alpha(t,x;)$ from (2.6) satisfy the following propagator (see, e.g., [20, 22]):

$$\begin{aligned} \frac{\partial\varphi_\alpha(t,x;u_0)}{\partial t} &= \mathcal{L}\varphi_\alpha(t,x;u_0) + \sum_{k=1}^q\sum_{l=1}^{\mathsf{n}}\alpha_{k,l}m_l(s)\mathcal{M}_k\varphi_{\alpha^-(k,l)}(x;u_0), \quad s\in(0,T],\\ \varphi_\alpha(0,x) &= u_0(x)\mathbf{1}_{\{|\alpha|=0\}}, \end{aligned}$$

where $\alpha^-(k,l)$ is the multi-index with components

$$\left(\alpha^-(k,l)\right)_{i,j} = \begin{cases}\max(0,\alpha_{i,j}-1) & \text{if } i=k \text{ and } j=l,\\ \alpha_{i,j} & \text{otherwise.}\end{cases} \tag{2.10}$$

In practical computations, we have to truncate the propagator (2.10) and, consequently, we are interested in the following truncated Wiener chaos solution:

$$u_{\mathsf{N},\mathsf{n}}(t,x) = \sum_{\alpha\in\mathcal{J}_{\mathsf{N},\mathsf{n},q}}\frac{1}{\sqrt{\alpha!}}\varphi_\alpha(t,x;u_0)\xi_\alpha, \tag{2.11}$$

FIG. 1. *Illustration of the idea of recursive multi-stage approach for long-time integration in* [37].

where the set $\mathcal{J}_{\mathsf{N},\mathsf{n},q} = \left\{\alpha = (\alpha_{k,l})_{q\times\mathsf{n}} | \sum_{k=1}^{q}\sum_{l=1}^{\mathsf{n}} \alpha_{k,l} \le \mathsf{N}\right\}$. Here N is the highest Hermite polynomial order and n is the maximum number of Gaussian random variables for each Wiener process. In (2.7), we choose the basis $\{m_l(s)\}_{l\ge 1}$ as

$$m_1(s) = \frac{1}{\sqrt{T}}, \quad m_l(s) = \sqrt{\frac{2}{T}}\cos\left(\frac{\pi(l-1)s}{T}\right), \quad l \ge 2, \quad 0 \le s \le T. \tag{2.12}$$

As shown in [4, 21, 37], the error induced by the truncation of WCE grows exponentially with time and thus WCE is not efficient for long-time integration. To control the error behavior, [37] proposes a recursive WCE (see Algorithm 2.1 below) for computing the second moments, $\mathbb{E}[u^2(t,x)]$, of the solution of the SPDE (2.1). Specifically, we discretize the Brownian motion using the following spectral representation in a multielement version, i.e., using K multielements [21, 37]:

$$w^{(\Delta,\mathsf{n})}(t) = \sum_{k=1}^{\mathsf{K}}\sum_{i=1}^{\mathsf{n}}\int_{\mathsf{t}_{k-1}\wedge t}^{\mathsf{t}_k\wedge t} m_{i,k}(s)\,ds\xi_{i,k}, \ t \in [0,T], \tag{2.13}$$

where $0 = \mathsf{t}_0 < \mathsf{t}_1 < \cdots < \mathsf{t}_\mathsf{K} = T$, $\mathsf{t}_k \wedge t$ is the minimum of $\mathsf{t}_k = k\Delta$ and t, $\{m_{i,k}\}_{i=1}^{\infty}$ is a CONS in $L^2([\mathsf{t}_k, \mathsf{t}_{k+1}])$, and $\xi_{i,k}$ are mutually independent standard Gaussian random variables. After the truncation of Brownian motion, we can have a similar propagator as (2.10). Noticing the linear property and Markovian properties of the solution to (2.1), we take the solution at t_{k-1} as an initial condition to solve the solution over $(\mathsf{t}_{k-1}, \mathsf{t}_k]$. Thus, we can recursively compute the covariance matrix at t_k with the covariance matrix at the time instant t_{k-1}. We then have the following algorithm for the second moments of the approximate solution; see Figure 1 for an illustration and [37] for the derivation.

ALGORITHM 2.1 (recursive multistage WCE [37, Algorithm 2]). *Choose the algorithm's parameters: a CONS $\{e_m(x)\}_{m\ge 1}$ and its truncation $\{e_m(x)\}_{m=1}^{\mathsf{M}}$; a time step Δ; and N and n, which together with the number of noises q determine the size of the multi-index set $\mathcal{J}_{\mathsf{N},\mathsf{n},q}$.*

Step 1. For each $m = 1, \ldots, \mathsf{M}$, solve the propagator (2.10) for $\alpha \in \mathcal{J}_{\mathsf{N},\mathsf{n},q}$ on the time interval $[0,\Delta]$ with the initial condition $\phi(x) = e_m(x)$ and denote the obtained solution as $\varphi_\alpha(\Delta, x; e_m)$, $m = 1, \ldots, \mathsf{M}$, and $\alpha \in \mathcal{J}_{\mathsf{N},\mathsf{n},q}$ Also, choose a time step size δt to solve numerically the equations in the propagator.

Step 2. Evaluate $q_{\alpha,l,m} = (\varphi_\alpha(\Delta,\cdot;e_l), e_m(\cdot))$, $l,m = 1,\ldots,\mathsf{M}$. Here $(\cdot,\cdot)$ is the inner product in $L^2(\mathcal{D})$.

Step 3. Recursively compute the covariance matrices $Q_{lm}(\mathsf{t}_i;\mathsf{N},\mathsf{n},\mathsf{M})$, $l,m = 1,\ldots,\mathsf{M}$, $\mathsf{t}_i = i\Delta$, as follows:

$$Q_{lm}(0;\mathsf{N},\mathsf{n},\mathsf{M}) = (u_0, e_l)(u_0, e_m),$$

$$Q_{lm}(\mathsf{t}_i;\mathsf{N},\mathsf{n},\mathsf{M}) = \sum_{j,k=1}^{\mathsf{M}} Q_{jk}(\mathsf{t}_{i-1};\mathsf{N},\mathsf{n},\mathsf{M}) \sum_{\alpha\in\mathcal{J}_{\mathsf{N},\mathsf{n},q}} \frac{1}{\alpha!} q_{\alpha,j,l}\, q_{\alpha,k,m}, \ i = 1,\ldots,\mathsf{K},$$

where $u_0(x)$ is the initial condition for (2.1), and obtain $\mathbb{M}^{\mathsf{M}}_{\Delta,\mathsf{N},\mathsf{n}}(\mathsf{t}_i, x)$, the second moments of the approximate solution to (2.1) by the following:

$$\mathbb{M}^{\mathsf{M}}_{\Delta,\mathsf{N},\mathsf{n}}(\mathsf{t}_i, x) = \sum_{l,m=1}^{\mathsf{M}} Q_{lm}(\mathsf{t}_i; \mathsf{N}, \mathsf{n}, \mathsf{M}) e_l(x) e_m(x), \; i = 1, \ldots, \mathsf{K}. \tag{2.14}$$

Remark 2.2. The complexity of this algorithm is of order M^4 but can be reduced to the order of M^2 by making full use of the sparsity of the data [37].

2.2. SCM. This method leads to a fully decoupled system instead of a weakly coupled system from the WCE. First, we rewrite the SPDE (2.1) in the Stratonovich form (see e.g., [13, 19]),

$$\begin{aligned} du(t,x) &= \tilde{\mathcal{L}} u(t,x)\, dt + \sum_{k=1}^{q} \mathcal{M}_k u(t,x) \circ dw_k(t), \; (t,x) \in (0,T] \times \mathcal{D}, \\ u(0,x) &= u_0(x), \quad x \in \mathcal{D}, \end{aligned} \tag{2.15}$$

where $\tilde{\mathcal{L}} u = \mathcal{L} u - \frac{1}{2} \sum_{1 \le k \le q} \mathcal{M}_k \mathcal{M}_k u$. Second, we approximate the Brownian motion with its multielement spectral expansion (2.13) and obtain the following partial differential equation with smooth random inputs (see, e.g., [13]):

$$\begin{aligned} d\tilde{u}_{\Delta,\mathsf{n}}(t,x) &= \tilde{\mathcal{L}} \tilde{u}_{\Delta,\mathsf{n}}(t,x)\, dt + \sum_{k=1}^{q} \mathcal{M}_k \tilde{u}_{\Delta,\mathsf{n}}(t,x) dw_k^{(\Delta,\mathsf{n})}(t), \; (t,x) \in (0,T] \times \mathcal{D}, \\ \tilde{u}(0,x) &= u_0(x), \quad x \in \mathcal{D}. \end{aligned} \tag{2.16}$$

In (2.16), we have $\mathsf{n}q\mathsf{K}$ standard Gaussian random variables $\xi_{l,k,i}$, $l \le \mathsf{n}, k \le q$, $i \le \mathsf{K}$, according to (2.13). Now we can apply standard numerical techniques of $\mathsf{n}q\mathsf{K}$-dimensional integration to numerically obtain pth moments of the solution to (2.16):

$$\mathbb{E}[(\tilde{u}_{\Delta,\mathsf{n}}(T,x))^p] = \frac{1}{(2\pi)^{\mathsf{n}q\mathsf{K}/2}} \int_{\mathbb{R}^{\mathsf{n}q\mathsf{K}}} \big(F(u_0(x), T, x, \mathbf{y})\big)^p e^{-\frac{\mathbf{y}^\top \mathbf{y}}{2}}\, d\mathbf{y}, \quad p = 1, 2, \ldots, \tag{2.17}$$

where $\mathbf{y} = (y_{l,k,i})$, $l \le \mathsf{n}, k \le q$, $i \le \mathsf{K}$, and the functional F represents the solution functional for (2.16). Here we use sparse grid collocation [12, 33] if the dimension $\mathsf{n}q\mathsf{K}$ is moderately large. As pointed out in [2, 36], we are led to a fully *decoupled* system of equations as in the case of Monte Carlo methods.

In practice, we use the following sparse grid quadrature rule for a d-dimensional function φ (see, e.g., [12, 33]):

$$A(\mathsf{L}, d)\varphi = \sum_{\mathsf{L} \le |\mathbf{i}| \le \mathsf{L}+d-1} (-1)^{\mathsf{L}+d-1-|\mathbf{i}|} \binom{d-1}{|\mathbf{i}| - \mathsf{L}} Q_{i_1} \otimes \cdots \otimes Q_{i_d} \varphi, \tag{2.18}$$

where we have one-dimensional Gauss–Hermite quadrature rules Q_n for univariate functions $\psi(\mathsf{y})$, $\mathsf{y} \in \mathbb{R}$: $Q_n \psi(\mathsf{y}) = \sum_{\alpha=1}^{n} \psi(\mathsf{y}_{n,\alpha}) \mathsf{w}_{n,\alpha}$, $\mathsf{y}_{n,1} < \mathsf{y}_{n,2} < \cdots < \mathsf{y}_{n,n}$ are the roots of the nth Hermite polynomial (2.8), and $\mathsf{w}_{n,\alpha}$ are the associated weights $\mathsf{w}_{n,\alpha} = n!/n^2 [H_{n-1}(\mathsf{y}_{n,\alpha})]^2$. The number of sparse grid points, denoted by $\eta(\mathsf{L}, d)$, for this sparse grid quadrature rule is of order $d^{\mathsf{L}-1}$ when $\mathsf{L} \le d$, which can be checked readily from the rule (2.18). For example, we have, for $\mathsf{L} = 2, 3, 4$,

$$\eta(2,d) = 2d + 1, \; \eta(3,d) = 2d^2 + 2d + 1, \; \eta(4,d) = \frac{4}{3} d^3 + 2d^2 + \frac{14}{3} d + 1.$$

Denote the set of $\eta(\mathsf{L}, d)$ sparse grid points $\mathsf{x}_\kappa = (\mathsf{x}_\kappa^1, \dots, \mathsf{x}_\kappa^d)$ by $\mathcal{H}_\mathsf{L}^{\mathsf{n}q}$, where x_κ^j $(1 \leq j \leq d)$ belongs to the set of points used by the quadrature rule Q_{i_j}. According to (2.18), we only need to know the function values at the sparse grid $\mathcal{H}_\mathsf{L}^{\mathsf{n}q}$:

$$A(\mathsf{L}, d)\varphi = \sum_{\kappa=1}^{\eta(\mathsf{L},\mathsf{n}q)} \varphi(\mathsf{x}_\kappa)\mathsf{W}_\kappa, \quad \mathsf{x}_\kappa = (\mathsf{x}_\kappa^1, \dots, \mathsf{x}_\kappa^d) \in \mathcal{H}_\mathsf{L}^{\mathsf{n}q}, \tag{2.19}$$

where W_κ are determined by (2.18) and the choice of the quadrature rules Q_{i_j} and they are called the sparse grid quadrature weights.

Here again, the direct application of SCM is efficient only for short-time integration. To achieve long-time integration, we apply the recursive multistage idea used in Algorithm 2.1, i.e., we use SCM over small time interval $(\mathsf{t}_{i-1}, \mathsf{t}_i]$ instead of over the whole interval $(0, T]$ and compute the second-order moments of the solution recursively in time. The derivation of such a recursive algorithm will make use of properties of the problem (2.1) and orthogonality of the basis both in physical space and in random space, as will be shown shortly.

We solve (2.16) with spectral methods in physical space, i.e., using a truncation of a CONS in physical space $\{e_m\}_{m=1}^{\mathsf{M}}$ to represent the numerical solution. The corresponding approximation of $\tilde{u}_{\Delta,\mathsf{n}}(t, x)$ is denoted by $\tilde{u}_{\Delta,\mathsf{n}}^{\mathsf{M}}(t, x)$. Further, let $v(t, x; s, v_0)$ be the approximation $\tilde{u}_{\Delta,\mathsf{n}}^{\mathsf{M}}(t, x)$ of $\tilde{u}_{\Delta,\mathsf{n}}(t, x)$ with the initial data v_0 prescribed at s: $\tilde{u}_{\Delta,\mathsf{n}}(s, x) = v_0(x)$. Note that

$$\tilde{u}_{\Delta,\mathsf{n}}^{\mathsf{M}}(\mathsf{t}_i, x) = v(\mathsf{t}_i, x; \mathsf{t}_{i-1}, \tilde{u}_{\Delta,\mathsf{n}}^{\mathsf{M}}(\mathsf{t}_{i-1}, \cdot)), \quad t_i = i\Delta. \tag{2.20}$$

Denote $\Phi_m(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M}) = (\tilde{u}_{\Delta,\mathsf{n}}^{\mathsf{M}}(\mathsf{t}_i, \cdot), e_m)$. Then the second moments are computed by

$$\mathbb{E}[(\tilde{u}_{\Delta,\mathsf{n}}^{\mathsf{M}}(\mathsf{t}_i, x))^2] = \sum_{l,m=1}^{\mathsf{M}} H_{lm}(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M}) e_l(x) e_m(x), \tag{2.21}$$

where $H_{lm}(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M}) = \mathbb{E}[\Phi_l(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M})\Phi_m(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M})]$. Now we show how the matrix $H_{lm}(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M})$ can be computed recursively. By the linearity of (2.16), we have

$$\tilde{u}_{\Delta,\mathsf{n}}^{\mathsf{M}}(\mathsf{t}_i, x) = \sum_{l=1}^{\mathsf{M}} \Phi_l(\mathsf{t}_{i-1}; \Delta, \mathsf{n}, \mathsf{M}) v(\mathsf{t}_i, x; \mathsf{t}_{i-1}, e_l).$$

Denote $h_{l,m,i-1} = (v(\mathsf{t}_i, \cdot; \mathsf{t}_{i-1}, e_l), e_m)$. Then by the orthonormality of e_m, we have

$$\Phi_m(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M}) = \sum_{l=1}^{\mathsf{M}} \Phi_l(\mathsf{t}_{i-1}; \Delta, \mathsf{n}, \mathsf{M}) h_{l,m,i-1}.$$

The matrix $H_{lm}(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M})$ can be computed recursively as

$$H_{lm}(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M}) = \sum_{j=1}^{\mathsf{M}} \sum_{k=1}^{\mathsf{M}} H_{jk}(\mathsf{t}_{i-1}; \Delta, \mathsf{n}, \mathsf{M}) \mathbb{E}[h_{j,l,i-1} h_{k,m,i-1}].$$

We note that the expectation $\mathbb{E}[h_{j,l,i-1} h_{k,m,i-1}]$ does not depend on $i-1$ because according to (2.16) and (2.2), $v(\mathsf{t}_i, x; \mathsf{t}_{i-1}, e_l)$ depends on the length of the time interval Δ and the random variables $\xi_{l,k,i}$ $(l \leq \mathsf{n},\ k \leq q)$ but is independent of time

t_{i-1}. Denote $v(\mathsf{t}_i, \cdot; \mathsf{t}_{i-1}, e_l)$ with $\xi_{l,k,i}$ anchored at the sparse grid point $\mathsf{x}_\kappa \in \mathcal{H}_{\mathsf{L}}^{\mathsf{n}q}$ by $\upsilon_\kappa(\Delta, \cdot; e_l)$. Let $h_{\kappa,l,m} = (\upsilon_\kappa(\Delta, \cdot; e_l), e_m)$. Then, using the sparse grid quadrature rule (2.19), we obtain the recursive approximation of $H_{lm}(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M})$:

$$H_{lm}(\mathsf{t}_i; \Delta, \mathsf{n}, \mathsf{M}) \approx H_{lm}(\mathsf{t}_i; \Delta, \mathsf{L}, \mathsf{n}, \mathsf{M}) := \sum_{j=1}^{\mathsf{M}} \sum_{k=1}^{\mathsf{M}} H_{jk}(\mathsf{t}_{i-1}; \Delta, \mathsf{L}, \mathsf{n}, \mathsf{M}) \sum_{\kappa=1}^{\eta(\mathsf{L},\mathsf{n}q)} h_{\kappa,j,l} h_{\kappa,k,m} \mathsf{W}_\kappa. \tag{2.22}$$

Substituting (2.22) in (2.21), we obtain an approximation for the second moments of $u(t, x)$, denoted by $\mathbb{M}^{\mathsf{M}}_{\Delta,\mathsf{L},\mathsf{n}}(\mathsf{t}_i, x)$. When $\mathsf{M} = \infty$ (i.e., when the CONS $\{e_m\}$ is not cut off), we denote this approximation by $\mathbb{M}_{\Delta,\mathsf{L},\mathsf{n}}(\mathsf{t}_i, x)$.

Remark 2.3. For nonhomogeneous equations, i.e., with forcing terms, we can have similar algorithms. Indeed, the same procedure applies once we can split the nonhomogeneous equations into two equations: a nonhomogeneous equation with zero initial value and a homogeneous equation with initial value. See [38] for a derivation of similar algorithms where only increments of Brownian motion are used, which is different from the spectral approximation of Brownian motion used here.

Now we have the following algorithm for the second moments of the approximate solution.

ALGORITHM 2.2 (recursive multistage SCM). *Choose a CONS* $\{e_m(x)\}_{m\geq 1}$ *and its truncation* $\{e_m(x)\}_{m=1}^{\mathsf{M}}$*; a time step* Δ*; and the sparse grid level* L *and* n*, which together with the number of noises* q *determine the sparse grid* $\mathcal{H}_{\mathsf{L}}^{\mathsf{n}q}$ *which contains* $\eta(\mathsf{L}, \mathsf{n}q)$ *sparse grid points.*

Step 1. For each $m = 1, \ldots, \mathsf{M}$, solve the system of equations (2.16) on the sparse grid $\mathcal{H}_{\mathsf{L}}^{\mathsf{n}q}$ in the time interval $[0, \Delta]$ with the initial condition $\phi(x) = e_m(x)$ and denote the obtained solution as $\upsilon_\kappa(\Delta, x; e_m)$, $m = 1, \ldots, \mathsf{M}$, and $\kappa = 1, \ldots, \eta(\mathsf{L}, \mathsf{n}q)$. Also, choose a time step size δt to solve (2.16) numerically.

Step 2. Evaluate $h_{\kappa,l,m} = (\upsilon_\kappa(\Delta, \cdot; e_l), e_m)$, $l, m = 1, \ldots, \mathsf{M}$.

Step 3. Recursively compute the covariance matrices $H_{lm}(\mathsf{t}_i; \mathsf{L}, \mathsf{n}, \mathsf{M})$, $l, m = 1, \ldots, \mathsf{M}$, as

$$H_{lm}(0; \Delta, \mathsf{L}, \mathsf{n}, \mathsf{M}) = (u_0, e_l)(u_0, e_m),$$
$$H_{lm}(\mathsf{t}_i; \Delta, \mathsf{L}, \mathsf{n}, \mathsf{M}) = \sum_{j,k=1}^{\mathsf{M}} H_{jk}(\mathsf{t}_{i-1}; \Delta, \mathsf{L}, \mathsf{n}, \mathsf{M}) \sum_{\kappa=1}^{\eta(\mathsf{L},\mathsf{n}q)} h_{\kappa,j,l} h_{\kappa,k,m} \mathsf{W}_\kappa, \; i = 1, \ldots, \mathsf{K},$$

where $u_0(x)$ is the initial condition for (2.1), and obtain the approximate second moments $\mathbb{M}^{\mathsf{M}}_{\Delta,\mathsf{L},\mathsf{n}}(\mathsf{t}_i, x)$ of the solution $u(t, x)$ to (2.1) as

$$\mathbb{M}^{\mathsf{M}(\mathsf{t}_i,x)}_{\Delta,\mathsf{L},\mathsf{n}} = \sum_{l,m=1}^{\mathsf{M}} H_{lm}(\mathsf{t}_i; \Delta, \mathsf{L}, \mathsf{n}, \mathsf{M}) e_l(x) e_m(x), \; i = 1, \ldots, \mathsf{K}. \tag{2.23}$$

Remark 2.4. Similar to Algorithm 2.1, the cost of this algorithm is $\frac{T}{\Delta}\eta(\mathsf{L}, \mathsf{n}q)\mathsf{M}^4$ and the storage is $\eta(\mathsf{L}, \mathsf{n}q)\mathsf{M}^2$. The total cost can be reduced to the order of M^2 by adopting reduced-order methods in physical space; see e.g., [32]. The discussion on computational efficiency of the recursive WCE methods (see [37, Remark 4.1]) is also valid for Algorithm 2.2.

3. Error estimates. Though WCE and SCM use the same spectral truncation of Brownian motion, the former is associated with the Ito–Wick product, while the latter is related to the Stratonovich product. Note that WCE employs orthogonal polynomials as a basis and SCM does not have such orthogonality. This difference allows WCE to have a better convergence rate than SCM in the second-order moments; see Corollary 3.2 and Theorem 3.3.

Assume that the operator $\mathcal{L}$ generates a semigroup $\{\mathcal{T}_t\}_{t\geq 0}$, which has the following properties: for $v \in H^k(\mathcal{D})$,

$$\left\|\mathcal{T}_t v\right\|_{H^k}^2 \leq C(k,\mathcal{L}) e^{2C_{\mathcal{L}}t}\left\|v\right\|_{H^k}^2, \tag{3.1}$$

where $C(0,\mathcal{L}) = 1$ and

$$\int_s^t e^{2C_{\mathcal{L}}(t-\theta)}\left\|\mathcal{T}_t v\right\|_{H^{k+1}}^2 d\theta \leq \delta_{\mathcal{L}}^{-1} C(k,\mathcal{L}) e^{2C_{\mathcal{L}}(t-s)}\left\|v\right\|_{H^k}^2. \tag{3.2}$$

Also, we assume that there exists a constant $\tilde{C}(r,\mathcal{M})$ such that

$$\left\|\mathcal{M}_l v\right\|_{H^k}^2 \leq \tilde{C}(k,\mathcal{M})\left\|v\right\|_{H^{k+1}}^2 \quad \text{for } v \in H^{k+1},\ l = 1,\ldots,q, \tag{3.3}$$

and that there exists a constant $\tilde{C}(k,\mathcal{L})$ such that

$$\left\|\mathcal{L}v\right\|_{H^k}^2 \leq \tilde{C}(k,\mathcal{L})\left\|v\right\|_{H^{k+2}}^2 \text{ for } v \in H^{k+2}. \tag{3.4}$$

The conditions (3.1) and (3.3) are satisfied with $k \leq r$ and (3.4) is satisfied with $k \leq r-1$ when the coefficients from (2.2) belong to the Hölder space $\mathcal{C}_b^{r+1}(\mathcal{D})$, which is equipped with the norm

$$\left\|f\right\|_{C_b^r} = \max_{0\leq|\beta|\leq\lfloor r\rfloor}\left\|D_\beta f\right\|_{L^\infty} + \sup_{\substack{x,y\in\mathcal{D}\\ |\beta|=\lfloor r\rfloor, r>\lfloor r\rfloor}} \frac{|D_\beta f(x) - D_\beta f(y)|}{|x-y|^{r-\lfloor r\rfloor}},$$

and $\lfloor r\rfloor$ is the integer part of the positive number r; cf. [11, section 5.1]. Define also

$$C_k = \max_{1\leq j\leq k}\left\{C(j,\mathcal{L})\tilde{C}(j-1,\mathcal{M})\right\}. \tag{3.5}$$

For the WCE for the SPDE (2.1) with single noise ($q=1$), we have the convergence results stated below. In the general case, we have not succeeded in proving such theorems but we numerically check convergence orders using examples with commutative noises and noncommutative noises in section 4.

THEOREM 3.1. *Let $q = 1$ in (2.1). Assume that $\sigma_{i,1}, a_{i,j}, b_i, c, \nu_1$ in (2.2) belong to $\mathcal{C}_b^{r+1}(\mathcal{D})$ and $u_0 \in H^r(\mathcal{D})$, where $r \geq \mathsf{N}+2$ and N is the order of Wiener chaos. Also assume that (2.3) holds. Then for $C_1 < \delta_{\mathcal{L}}$, the error of the truncated Wiener chaos solution $u_{\mathsf{N},\mathsf{n}}(\mathsf{t}_i,x)$ from (2.11) is estimated as*

$$\begin{aligned}
&(\mathbb{E}[\left\|u_{\mathsf{N},\mathsf{n}}(\mathsf{t}_i,\cdot) - u(\mathsf{t}_i,\cdot)\right\|^2])^{1/2} \\
&\quad\leq (C_{\lfloor r\rfloor}\Delta)^{\mathsf{N}/2} e^{C_{\mathcal{L}}T}\left[\frac{e^{C_{\lfloor r\rfloor}T}}{(\mathsf{N}+1)!} + \frac{(C_{\lfloor r\rfloor}\Delta)^{\lfloor r\rfloor-\mathsf{N}-1}}{\lfloor r\rfloor!}\frac{\delta_{\mathcal{L}}}{\delta_{\mathcal{L}}-C_1}\right]^{1/2}\left\|u_0\right\|_{H^r} \\
&\qquad + \sqrt{2C_{\mathsf{N}+2}C(\mathsf{N}+2,\mathcal{L})\tilde{C}(\mathsf{N},\mathcal{L})}\, e^{C_{\mathsf{N}+2}T + C_{\mathcal{L}}T}\frac{\Delta}{\sqrt{\mathsf{n}}\pi}\left\|u_0\right\|_{H^{\mathsf{N}+2}},
\end{aligned} \tag{3.6}$$

where $\mathsf{t}_i = i\Delta$, the constants $\delta_{\mathcal{L}}$ and $C_{\mathcal{L}}$ are from (2.3), $C_{\lfloor r\rfloor}$ is defined in (3.5), $\tilde{C}(\mathsf{N},\mathcal{L})$ is from (3.4), and $C(\mathsf{N}+2,\mathcal{L})$ is from (3.1).

From Theorem 3.1, we have that the mean-square error of the recursive multi-stage WCE is $\mathcal{O}(\Delta^{\mathsf{N}/2}) + \mathcal{O}(\Delta)$. The same result is proved for $q = 1$ and $\sigma_{i,r} = 0$ in [21], where the condition $C_1 < \delta_{\mathcal{L}}$ is not required. Also, for the case of $\sigma_{i,r} \neq 0$, the mean-square convergence without order but not requiring the condition $C_1 < \delta_{\mathcal{L}}$ was proved in [20, 22].

Corollary 3.2. *Under the assumptions of Theorem* 3.1*, we have*

$$\begin{aligned}
&\left|\mathbb{E}[\left\|u_{\mathsf{N},\mathsf{n}}(\mathsf{t}_i,\cdot)\right\|^2] - \mathbb{E}[\left\|u(\mathsf{t}_i,\cdot)\right\|^2]\right| = \mathbb{E}[\left\|u_{\mathsf{N},\mathsf{n}}(\mathsf{t}_i,\cdot) - u(\mathsf{t}_i,\cdot)\right\|^2] \\
&\quad\le (C_{\lfloor r\rfloor}\Delta)^{\mathsf{N}} e^{2C_{\mathcal{L}}T}\left[\frac{e^{C_{\lfloor r\rfloor}T}}{(\mathsf{N}+1)!} + \frac{(C_{\lfloor r\rfloor}\Delta)^{\lfloor r\rfloor-\mathsf{N}-1}}{\lfloor r\rfloor!}\frac{\delta_{\mathcal{L}}}{\delta_{\mathcal{L}}-C_1}\right]\left\|u_0\right\|^2_{H^r} \\
&\qquad + 2C_{\mathsf{N}+2}C(\mathsf{N}+2,\mathcal{L})\tilde{C}(\mathsf{N},\mathcal{L})e^{2C_{\mathsf{N}+2}T+2C_{\mathcal{L}}T}\frac{\Delta^2}{\mathsf{n}\pi^2}\left\|u_0\right\|^2_{H^{\mathsf{N}+2}}.
\end{aligned} \tag{3.7}$$

This corollary states that the convergence rate of the error in second-order moments (3.7) is twice that of the mean-square error (3.6), i.e., $\mathcal{O}(\Delta^{\mathsf{N}}) + \mathcal{O}(\Delta^2)$. This corollary can be proved by the orthogonality of WCE. In fact, it holds that

$$\mathbb{E}[u^2(\mathsf{t}_i,x)] - \mathbb{E}[u^2_{\mathsf{N},\mathsf{n}}(\mathsf{t}_i,x)] = \mathbb{E}[(u(\mathsf{t}_i,x) - u_{\mathsf{N},\mathsf{n}}(\mathsf{t}_i,x))^2], \tag{3.8}$$

as the different terms in the Cameron–Martin basis are mutually orthogonal [6]. Then by integration over the physical domain and by the Fubini theorem, we reach the conclusion in theorem 3.1.

For SCM for the SPDE (2.1), we have the following estimates: the first one is weak convergence of the Wong–Zakai type approximation $\tilde{u}_{\Delta,\mathsf{n}}(t,x)$ from (2.16) to $u(t,x)$ from (2.1) (see Theorem 3.3); the second one is the convergence of SCM, i.e., the convergence of $\mathbb{M}_{\Delta,\mathsf{L},\mathsf{n}}(\mathsf{t}_i,x)$ to $\mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{n}}(\mathsf{t}_i,x)]$ (see Theorem 3.4). Here we prove the convergence rate when $\sigma_{i,r} = 0$, which belongs to the case of commutative noises (2.4). Our proof for Theorem 3.3 is based on the mean-square of convergence of the Wong–Zakai type approximation (2.16) to (2.1). When $\sigma_{i,r} \neq 0$, we have not succeeded in proving this mean-square convergence and, as far as we know, only a rate of almost sure convergence of the Wong–Zakai type approximations to (2.1) has been proved so far [13].

Theorem 3.3. *Assume that $\sigma_{i,r} = 0$ and that the initial condition u_0 and the coefficients in* (2.2) *are in $\mathcal{C}^2_b(\mathcal{D})$. Let $u(t,x)$ be the solution to* (2.1) *and $\tilde{u}_{\Delta,\mathsf{n}}(t,x)$ be the solution to* (2.16)*. Then for any $\varepsilon > 0$, there exists a constant $C > 0$ such that the one-step error is estimated by*

$$\left|\mathbb{E}[u^2(\Delta,x)] - \mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x)]\right| \le C\exp(C\Delta)(\Delta^6 + \Delta^2)\mathsf{n}^{-1+\varepsilon}, \tag{3.9}$$

and the global error is estimated by

$$\left|\mathbb{E}[u^2(\mathsf{t}_i,x)] - \mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{n}}(\mathsf{t}_i,x)]\right| \le C\exp(CT)\Delta\mathsf{n}^{-1+\varepsilon}, \quad 1 \le i \le \mathsf{K}. \tag{3.10}$$

The following theorem is on the convergence of the second moments by SCM to those of the solution to (2.16).

Theorem 3.4. *Let $\tilde{u}_{\Delta,\mathsf{n}}(t,x)$ be the solution to* (2.16) *and $\mathbb{M}_{\Delta,\mathsf{L},\mathsf{n}}(\mathsf{t}_i,x)$be the limit of $\mathbb{M}^{\mathsf{M}}_{\Delta,\mathsf{L},\mathsf{n}}(\mathsf{t}_i,x)$ from* (2.23) *when $\mathsf{M} \to \infty$. Under the assumptions of Theorem* 3.3*, for any $\varepsilon > 0$, the one-step error is estimated by*

$$\begin{aligned}
&\left|\mathbb{M}_{\Delta,\mathsf{L},\mathsf{n}}(\Delta,x) - \mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x)]\right| \\
&\quad\le C\exp(C\Delta)(\Delta^{3\mathsf{L}} + \Delta^{2\mathsf{L}})(1 + (3c/2)^{\mathsf{L}\wedge\mathsf{n}})\beta^{-(\mathsf{L}\wedge\mathsf{n})/2}\varepsilon^{-\mathsf{L}}\mathsf{L}^{-1}\mathsf{n}^{\mathsf{L}\varepsilon},
\end{aligned}$$

and the global error is estimated by, for $1 \le i \le \mathsf{K}$,

$$\left|\mathbb{M}_{\Delta,\mathsf{L},\mathsf{n}}(\mathsf{t}_i,x) - \mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{n}}(\mathsf{t}_i,x)]\right| \le C\exp(CT)\Delta^{2\mathsf{L}-1}(1+(3c/2)^{\mathsf{L}\wedge\mathsf{n}})\beta^{-(\mathsf{L}\wedge\mathsf{n})/2}\varepsilon^{-\mathsf{L}}\mathsf{L}^{-1}\mathsf{n}^{\mathsf{L}\varepsilon}.$$

Here the positive constants C, c, $\beta < 1$ *are independent of* Δ, L, *and* n. *The expression* $\mathsf{L}\wedge\mathsf{n}$ *means the minimum of* L *and* n.

According to Theorems 3.3 and 3.4, the error of the SCM is $\mathcal{O}(\Delta^{2\mathsf{L}-1}) + \mathcal{O}(\Delta)$ in the second-order moments. Compared to Corollary 3.2, the SCM is of one order lower than WCE when $\mathsf{N} = 2$ as the error of WCE is $\mathcal{O}(\Delta^{\mathsf{N}}) + \mathcal{O}(\Delta^2)$.

4. Numerical results. In this section, we compare Algorithms 2.1 and 2.2 for linear stochastic advection-diffusion-reaction equations with commutative and noncommutative noises. We will test the computational performance of these two methods in terms of accuracy and computational cost. All the tests were run using MATLAB R2012b, on a Macintosh desktop computer with Intel Xeon CPU E5462 (quad-core, 2.80 GHz). Every effort was made to program and execute the different algorithms as much as possible in an identical way.

We note that we do not have exact solutions for all examples and hence evaluate the errors of the second-order moments using reference solutions, denoted by $\mathbb{E}[u^2_{\mathrm{ref}}(T,x)]$, which are obtained by either Algorithm 2.1 or Algorithm 2.2 with fine resolution. We do not use solutions obtained from Monte Carlo methods as reference solutions since Monte Carlo methods are of low accuracy and are less accurate than the recursive multistage WCE; see [37] for a comparison between WCE and Monte Carlo methods, and also see below.

The following error measures are used in the numerical examples below:

$$\varrho^2_2(T) = \left|\left\|\mathbb{E}[u^2_{\mathrm{ref}}(T,\cdot)]\right\|_{l^2} - \left\|\mathbb{M}^{\mathsf{M}}_{\Delta}(T,\cdot)\right\|_{l^2}\right|, \quad \varrho^{r,2}_2(T) = \frac{\varrho^2_2(T)}{\left\|\mathbb{E}[u^2_{\mathrm{ref}}(T,\cdot)]\right\|_{l^2}}, \tag{4.1}$$

$$\varrho^{\infty}_2(T) = \left|\left\|\mathbb{E}[u^2_{\mathrm{ref}}(T,\cdot)]\right\|_{l^\infty} - \left\|\mathbb{M}^{\mathsf{M}}_{\Delta}(T,\cdot))\right\|_{l^\infty}\right|, \quad \varrho^{r,\infty}_2(T) = \frac{\varrho^{\infty}_2(T)}{\left\|\mathbb{E}[u^2_{\mathrm{ref}}(T,\cdot)]\right\|_{l^\infty}}, \tag{4.2}$$

where $\mathbb{M}^{\mathsf{M}}_{\Delta}(T,x)$ is either $\mathbb{M}^{\mathsf{M}}_{\Delta,\mathsf{N},\mathsf{n}}(T,x)$ from Algorithm 2.1 or $\mathbb{M}^{\mathsf{M}}_{\Delta,\mathsf{L},\mathsf{n}}(T,x)$ from Algorithm 2.2, $\left\|v\right\|_{l^2} = (\frac{2\pi}{\mathsf{M}}\sum_{m=1}^{\mathsf{M}} v^2(x_m))^{\frac{1}{2}}$, $\left\|v\right\|_{l^\infty} = \max_{1\le m\le \mathsf{M}} |v(x_m)|$, and x_m are the Fourier collocation points.

The computational complexity for Algorithm 2.1 is $\binom{\mathsf{N}+\mathsf{n}q}{\mathsf{N}}\frac{T}{\Delta}\mathsf{M}^4$ (see [37]) and that for Algorithm 2.2 is $\eta(\mathsf{L},\mathsf{n}q)\frac{T}{\Delta}\mathsf{M}^4$. The ratio of the computational cost of SCM over that of WCE is $\eta(\mathsf{L},\mathsf{n}q)/\binom{\mathsf{N}+\mathsf{n}q}{\mathsf{N}}$. For example, when $\mathsf{N} = 1$ and $\mathsf{L} = 2$, the ratio is $(1+2\mathsf{n}q)/(1+\mathsf{n}q)$, which will be used in the three numerical examples. The complexity increases exponentially with $\mathsf{n}q$ and L (see, e.g., [12]) or N but increases linearly with $\frac{T}{\Delta}$. Hence, we only consider low values of L and N.

Example 4.1 (single noise). We consider a single noise in the Ito SPDE (2.1) over the domain $(0,T]\times(0,2\pi)$,

$$du = \left[\left(\epsilon + \frac{1}{2}\sigma^2\right)\partial^2_x u + \beta\sin(x)\partial_x u\right]dt + \sigma\partial_x u\,dw(t), \tag{4.3}$$

or equivalently in the Stratonovich form,

$$du = [\epsilon\partial^2_x u + \beta\sin(x)\partial_x u]\,dt + \sigma\partial_x u \circ dw(t), \tag{4.4}$$

with periodic boundary conditions and nonrandom initial condition $u(0,x) = \cos(x)$, where $w(t)$ is a standard scalar Wiener process, and $\epsilon > 0$, β, σ are constants.

TABLE 1
Algorithm 2.1*: recursive multistage Wiener chaos method for* (4.3) *at* $T = 5$*:* $\sigma = 0.5$, $\beta = 0.1$, $\epsilon = 0.02$, *and* $\mathsf{M} = 20$, $\mathsf{n} = 1$.

Δ	δt	N	$\varrho_2^{r,2}(T)$	Order	$\varrho_2^{r,\infty}(T)$	Order	CPU time (sec.)
1.0e-1	1.0e-2	1	1.5249e-2	–	8.8177e-3		3.57
1.0e-2	1.0e-3	1	1.5865e-3	$\Delta^{0.98}$	8.9310e-4	$\Delta^{0.99}$	33.22
1.0e-3	1.0e-4	1	1.5934e-4	$\Delta^{1.00}$	8.9429e-5	$\Delta^{1.00}$	348.03
1.0e-1	1.0e-2	2	1.9070e-4	–	4.1855e-5	–	5.14
1.0e-2	1.0e-3	2	2.0088e-6	$\Delta^{1.98}$	4.2889e-7	$\Delta^{1.99}$	51.75
1.0e-3	1.0e-4	2	2.0386e-8	$\Delta^{1.99}$	4.8703e-9	$\Delta^{1.94}$	490.04

In this example, we compare Algorithms 2.1 and 2.2 for (4.3) with the parameters $\beta = 0.1$, $\sigma = 0.5$ and $\epsilon = 0.02$. We will show that the recursive multistage WCE is at most of order Δ^2 in the second-order moments and the recursive multistage SCM is of order Δ.

In Step 1, Algorithm 2.1, we employ the Crank–Nicolson scheme in time and Fourier collocation in physical space. We obtain the reference solution by Algorithm 2.1 with the same solver but finer resolution as a reference solution[1] since we have no exact solution to (4.3). The reference solution is obtained by $\mathsf{M} = 30$, $\Delta = 10^{-4}$, $\mathsf{N} = 4$, $\mathsf{n} = 4$, $\delta t = 10^{-5}$. It gives the second-order moments in l^2-norm $\left\|\mathbb{E}[u_{\mathrm{ref}}^2]\right\|_{l^2} \doteq 1.065194550063$ and in the l^∞-norm $\left\|\mathbb{E}[u_{\mathrm{ref}}^2]\right\|_{l^\infty} \doteq 0.5174746141105$.

From Table 1, we observe that the recursive WCE is $\mathcal{O}(\Delta^{\mathsf{N}}) + \mathcal{O}(\Delta^2)$ for the second-order moments. When $\mathsf{N} = 2$, the method is of second-order convergence in Δ and of first-order convergence when $\mathsf{N} = 1$. When $\mathsf{N} = 3$, the method is still second-order in Δ (not presented here). This verifies the estimate in Corollary 3.2.

In Step 1, Algorithm 2.2, we use the Crank–Nicolson scheme in time and Fourier collocation method in physical space. The errors are also measured as in (4.1) and (4.2). The reference solution is obtained by Algorithm 2.1 as in the case of WCE. We observe in Table 2 that the convergence order for second-order moments is one in Δ even when the sparse grid level L is 2, 3, and 4 (the last is not presented here). The errors for $\mathsf{L} = 3$ are more than half in magnitude smaller than those for $\mathsf{L} = 2$, while the time cost for $\mathsf{L} = 3$ is about 1.5 times of that for $\mathsf{L} = 2$.

In summary, from Tables 1 and 2, we observe that the recursive multistage WCE is $\mathcal{O}(\Delta^{\mathsf{N}}) + \mathcal{O}(\Delta^2)$ and the recursive multistage SCM is $\mathcal{O}(\Delta)$, as predicted by the error estimates in section 3. While the SCM and the WCE are of the same order when $\mathsf{N} = 1$ and $\mathsf{L} \geq 2$, the former can be more accurate than the latter. In fact, when $\mathsf{N} = 1$ and $\mathsf{L} = 2$, the recursive multistage SCM error is almost two orders of magnitude smaller than the recursive multistage WCE, while the computational cost for both is almost the same, as predicted ($\binom{\mathsf{N}+\mathsf{n}q}{\mathsf{N}} = \eta(\mathsf{L}, \mathsf{n}q) = 2$). The recursive multistage WCE with $\mathsf{N} = 2$ is of order Δ^2 and its errors are almost two orders of magnitude smaller than those by the recursive multistage SCM (with level 2 or 3) for the second-order moments.

[1]For single noise, it is proved in Theorem 3.1 that the recursive multistage WCE is of second-order convergence in second-order moments. The second-order convergence is numerically verified in [37]. For this specific example, a Monte Carlo method with 10^6 sampling paths (which costs 27.6 hours) gives $\left\|\mathbb{E}[u_{\mathrm{MC}}^2]\right\| = 1.06517 \pm 6.1 \times 10^{-4}$ and $\left\|\mathbb{E}[u_{\mathrm{MC}}^2]\right\|_\infty = 0.51746 \pm 6.1 \times 10^{-4}$, where the numbers after $\pm$ are the statistical errors with the 95% confidence interval. We use Fourier collocation in space with $M = 20$ and Crank–Nicolson in time with $\delta t = 10^{-3}$ for the Monte Carlo method.

Table 2

Algorithm 2.2*: recursive multistage SCM for* (4.3) *at* $T = 5$*:* $\sigma = 0.5$*,* $\beta = 0.1$*,* $\epsilon = 0.02$*, and* $\mathsf{M} = 20$*,* $\mathsf{n} = 1$.

Δ	δt	L	$\varrho_2^{r,2}(T)$	Order	$\varrho_2^{r,\infty}(T)$	Order	CPU time (sec.)
1e-01	1e-02	2	3.4808e-04	–	3.0383e-03	–	3.71
1e-02	1e-03	2	3.4839e-05	$\Delta^{1.00}$	3.0130e-04	$\Delta^{1.00}$	33.88
1e-03	1e-04	2	3.4844e-06	$\Delta^{1.00}$	3.0106e-05	$\Delta^{1.00}$	325.06
1e-01	1e-02	3	1.6815e-04	–	3.4829e-04	–	5.16
1e-02	1e-03	3	1.6230e-05	$\Delta^{1.02}$	3.2283e-05	$\Delta^{1.03}$	50.59
1e-03	1e-04	3	1.6170e-06	$\Delta^{1.00}$	3.2026e-06	$\Delta^{1.00}$	486.08

In this example, the recursive multistage SCM outperforms the recursive multistage WCE with $\mathsf{N} = 1$. The reason can be as follows. In SCM, we solve an advection-dominated equation rather than a diffusion-dominated equation in WCE, as SCM is associated with the Stratonovich product which leads to the removal of the term $\frac{1}{2}\sigma^2\partial_x^2 u$ in the resulting equation; see (4.4). The larger σ is, the more dominant the diffusion is. In fact, results for $\sigma = 1$ and $\sigma = 0.1$ (not presented here) show that when $\sigma = 1$, the relative error of SCM with $\mathsf{L} = 2$ is almost three orders of magnitude smaller than WCE with $\mathsf{N} = 1$; when $\sigma = 0.1$, the relative error of SCM with $\mathsf{L} = 2$ is only less than one order of magnitude smaller than WCE with $\mathsf{N} = 1$. With the Crank–Nicolson scheme in time and Fourier collocation in physical space, we cannot achieve better accuracy for WCE with $\mathsf{N} = 1$ and Δ no less than 0.0005 when $\mathsf{M} \leq 40$.

Example 4.2 (commutative noises). We consider two commutative noises in the Ito SPDE (2.1) over the domain $(0, T] \times (0, 2\pi)$,

$$\begin{aligned} du = &\left[\left(\epsilon + \frac{1}{2}\sigma_1^2\cos^2(x)\right)\partial_x^2 u + \left(\beta\sin(x) - \frac{1}{4}\sigma_1^2\sin(2x)\right)\partial_x u\right] dt \\ &+ \sigma_1\cos(x)\partial_x u\, dw_1(t) + \sigma_2 u\, dw_2(t), \end{aligned} \tag{4.5}$$

or equivalently in the Stratonovich form,

$$du = [\epsilon\partial_x^2 u + \beta\sin(x)\partial_x u]\, dt + \sigma_1\cos(x)\partial_x u \circ dw_1(t) + \sigma_2 u \circ dw_2(t), \tag{4.6}$$

with periodic boundary conditions and nonrandom initial condition $u(0, x) = \cos(x)$, where $(w_1(t), w_2(t))$ is a standard two-dimensional Wiener process, and $\epsilon > 0$, β, σ_1, σ_2 are constants. The problem has commutative noises; see (2.4).

In this example, we take $\sigma_1 = 0.5$, $\sigma_2 = 0.2$, $\beta = 0.1$, $\epsilon = 0.02$. We again observe first-order convergence for SCM and WCE with $\mathsf{N} = 1$ and second-order convergence for WCE with $\mathsf{N} = 2$ as in the last example with single noise.

We choose the same space-time solver for the recursive multistage WCE and SCM as in the last example. We compute the errors as in (4.1) and (4.2). In Table 3, the reference second moments are $\left\|\mathbb{M}^{\mathsf{M}}_{\Delta=10^{-4},\mathsf{N},\mathsf{n}}(T,\cdot))\right\|_{l^2}$ and $\left\|\mathbb{M}^{\mathsf{M}}_{\Delta=10^{-4},\mathsf{N},\mathsf{n}}(T,\cdot)\right\|_{l^\infty}$ obtained by Algorithm 2.1 with $\delta t = 10^{-5}$ and all the other truncation parameters are the same as stated in the table. In Table 4, the reference second moments are $\left\|\mathbb{M}^{\mathsf{M}}_{\Delta=10^{-4},\mathsf{L},\mathsf{n}}(T)\right\|_{l^2}$ and $\left\|\mathbb{M}^{\mathsf{M}}_{\Delta=10^{-4},\mathsf{L},\mathsf{n}}(T)\right\|_{l^\infty}$ obtained by Algorithm 2.2 with $\delta t = 10^{-5}$, while all the other truncation parameters are the same as in the table.

Here we do not compare the performance of Monte Carlo simulations with our algorithms as the main cost of Monte Carlo methods is to reduce the statistical errors. For the same parameters described above, when we used 10^6 Monte Carlo sampling

TABLE 3

Algorithm 2.1: recursive multistage WCE for commutative noises (4.5) at $T = 1$: $\sigma_1 = 0.5$, $\sigma_2 = 0.2$, $\beta = 0.1$, $\epsilon = 0.02$, and $\mathsf{M} = 30$, $\mathsf{n} = 1$.

Δ	δt	N	$\bar{\varrho}_2^{r,2}(T)$	Order	$\bar{\varrho}_2^{r,\infty}(T)$	Order	CPU time (sec.)
1e-01	1e-02	1	1.6994e-03	–	1.6548e-03	–	3.19
1e-02	1e-03	1	1.7838e-04	$\Delta^{0.98}$	1.7172e-04	$\Delta^{0.98}$	32.74
1e-03	1e-04	1	1.6323e-05	$\Delta^{1.04}$	1.5694e-05	$\Delta^{1.04}$	329.15
1e-01	1e-02	2	4.0658e-05	–	2.9568e-05	–	6.53
1e-02	1e-03	2	4.4805e-07	$\Delta^{1.96}$	3.3106e-07	$\Delta^{1.95}$	65.89
1e-03	1e-04	2	4.4682e-09	$\Delta^{2.00}$	3.3484e-09	$\Delta^{2.00}$	657.55

TABLE 4

Algorithm 2.2: recursive multistage SCM for commutative noises (4.5) at $T = 1$: $\sigma_1 = 0.5$, $\sigma_2 = 0.2$, $\beta = 0.1$, $\epsilon = 0.02$, and $\mathsf{M} = 30$, $\mathsf{n} = 1$.

Δ	δt	L	$\bar{\varrho}_2^{r,2}(T)$	Order	$\bar{\varrho}_2^{r,\infty}(T)$	Order	CPU time (sec.)
1e-01	1e-02	2	1.3624e-04	–	1.2453e-03	–	5.18
1e-02	1e-03	2	1.3064e-05	$\Delta^{1.02}$	1.2009e-04	$\Delta^{1.02}$	54.70
1e-03	1e-04	2	1.1837e-06	$\Delta^{1.04}$	1.0889e-05	$\Delta^{1.04}$	545.20
1e-01	1e-02	3	2.5946e-04	–	2.0482e-04	–	13.26
1e-02	1e-03	3	2.5437e-05	$\Delta^{1.01}$	1.7897e-05	$\Delta^{1.06}$	142.23
1e-03	1e-04	3	2.3102e-06	$\Delta^{1.04}$	1.6062e-06	$\Delta^{1.05}$	1420.24

paths, we could only reach the statistical error of 8.3×10^{-4}, in 3.9 hours. To obtain an error of 1×10^{-5}, 7000 times more Monte Carlo sampling paths should be used, requiring 3 years of computational time and thus not considered here. In the next example, we have similar situations and hence we will not consider Monte Carlo simulations. This also demonstrates the computational efficiency of Algorithms 2.1 and 2.2 in comparison with Monte Carlo methods.

For WCE, we observe in Table 3 convergence of order Δ^{N} ($\mathsf{N} \leq 2$) in the second-order moments: first-order convergence when $\mathsf{N} = 1$, and second-order convergence when $\mathsf{N} = 2$. Numerical results for $\mathsf{N} = 3$ (not presented here) show that the convergence order is still two even though the accuracy is further improved when N increases from 2 to 3. This is consistent with our estimate $\mathcal{O}(\Delta^{\mathsf{N}}) + \mathcal{O}(\Delta^2)$ in Corollary 3.2.

We also tested the case $\mathsf{n} = 2$, which gives similar results and the same convergence order.

For SCM, we observe first-order convergence in Δ from Table 4 when $\mathsf{L} = 2, 3$. We note that further refinements in truncation parameters in random space, i.e., increasing L and/or n, do not change the convergence order or improve the accuracy. The case $\mathsf{L} = 3$ actually leads to somewhat worse accuracy, compared with the case $\mathsf{L} = 2$. We tested the case $\mathsf{L} = 4$, which leads to the same magnitudes of errors as $\mathsf{L} = 3$. We also tested $\mathsf{n} = 2$ and observed no improved accuracy for $\mathsf{L} = 2, 3, 4$. These numerical results are not presented here.

For the two commutative noises, we conclude from this example that the recursive multistage WCE is of order $\Delta^{\mathsf{N}} + \Delta^2$ in the second-order moments and that the recursive multistage SCM is of order Δ in the second-order moments no matter what sparse grid level is used. The errors of recursive multistage SCM are one order of magnitude smaller than those of recursive multistage WCE with $\mathsf{N} = 1$, while the time cost of SCM is about 1.6 times of that cost of WCE. For large magnitude of

TABLE 5

Algorithm 2.1 *(recursive multistage WCE, left) and Algorithm* 2.2 *(recursive multistage SCM, right) for* (4.7) *at $T = 1$: $\sigma_1 = 0.5$, $\sigma_2 = 0.2$, $\beta = 0.1$, $\epsilon = 0.02$, and $\mathsf{M} = 20$, $\mathsf{n} = 1$. The time step size δt is $\Delta/10$. The reported CPU time is in seconds.*

Δ	N	$\bar{\varrho}_2^{r,2}(T)$	Order	Time (sec.)	L	$\bar{\varrho}_2^{r,2}(T)$	Order	Time (sec.)
1.0e-1	1	3.7516e-03	–	1.04	2	6.4343e-04	–	1.65
5.0e-2	1	1.8938e-03	$\Delta^{0.99}$	2.11	2	3.1738e-04	$\Delta^{1.02}$	3.31
2.0e-2	1	7.5292e-04	$\Delta^{1.01}$	5.12	2	1.2440e-04	$\Delta^{1.02}$	8.64
1.0e-2	1	3.6796e-04	$\Delta^{1.03}$	10.19	2	**6.0502e-05**	$\Delta^{1.04}$	**17.12**
5.0e-3	1	1.7457e-04	$\Delta^{1.08}$	20.01	2	2.8635e-05	$\Delta^{1.08}$	33.82
2.0e-3	1	**5.8246e-05**	$\Delta^{1.20}$	**50.39**	2	9.5401e-06	$\Delta^{1.12}$	86.44
1.0e-1	2	9.4415e-05	–	2.16	3	1.5803e-04	–	4.03
5.0e-2	2	**3.7303e-05**	$\Delta^{1.81}$	**4.11**	3	**7.6548e-05**	$\Delta^{1.05}$	**8.68**
2.0e-2	2	1.2282e-05	$\Delta^{1.34}$	9.97	3	2.9673e-05	$\Delta^{1.03}$	22.08
1.0e-2	2	5.5807e-06	$\Delta^{1.21}$	20.03	3	1.4378e-05	$\Delta^{1.05}$	43.85
5.0e-3	2	2.5471e-06	$\Delta^{1.14}$	40.25	3	6.7925e-06	$\Delta^{1.08}$	88.35
2.0e-3	2	8.2965e-07	$\Delta^{1.22}$	101.34	3	2.2605e-06	$\Delta^{1.20}$	223.15

noises ($\sigma_1 = \sigma_2 = 1$; numerical results are not presented), we observed that the SCM with $\mathsf{L} = 2$ and WCE with $\mathsf{N} = 1$ have the same order-of-magnitude accuracy. In this example, the use of SCM with $\mathsf{L} = 2$ for small magnitude of noises is competitive with the use of WCE with $\mathsf{N} = 1$.

Example 4.3 (noncommutative noises). We consider two noncommutative noises in the Ito SPDE (2.1) over the domain $(0, T] \times (0, 2\pi)$,

$$\begin{aligned} du = {} & \left[\left(\epsilon + \frac{1}{2}\sigma_1^2\right)\partial_x^2 u + \beta \sin(x)\partial_x u + \frac{1}{2}\sigma_2^2 \cos^2(x) u\right] dt \\ & + \sigma_1 \partial_x u \, dw_1(t) + \sigma_2 \cos(x) u \, dw_2(t), \end{aligned} \tag{4.7}$$

or equivalently in the Stratonovich form,

$$du = [\epsilon \partial_x^2 u + \beta \sin(x)\partial_x u]\, dt + \sigma_1 \partial_x u \circ dw_1(t) + \sigma_2 \cos(x) u \circ dw_2(t), \tag{4.8}$$

with periodic boundary conditions and nonrandom initial condition $u(0, x) = \cos(x)$, where $(w_1(t), w_2(t))$ is a standard Wiener process, and $\epsilon > 0$, β, σ_1, σ_2 are constants. The problem has noncommutative noises as the coefficients do not satisfy (2.4).

We take the same constants $\epsilon > 0$, β, σ_1, σ_2 as in the last example. We also take the same space-time solver as in the last example. In the current example, we observe only first-order convergence for SCM (level $\mathsf{L} = 2, 3, 4$) and WCE ($\mathsf{N} = 1, 2, 3$) when $\mathsf{n} = 1, 2$; see Table 5 for parts of the numerical results.

The errors are computed as in the last example. The reference solutions are obtained by Algorithm 2.1 for the recursive multistage WCE solutions and by Algorithm 2.2 for the recursive multistage SCM solutions, with $\Delta = 5 \times 10^{-4}$ and $\delta t = 5 \times 10^{-5}$ and all the other truncation parameters the same as stated in Tables 5 and 6.

In this example, our error estimate for recursive multistage WCE is not valid any more and the numerical results suggest that the errors behave as $\Delta^{\mathsf{N}} + C\Delta/\mathsf{n}$. For $\mathsf{N} = 1$ and $\mathsf{n} = 10$ (not presented), the error is almost the same as $\mathsf{n} = 1$. While $\mathsf{N} = 2$ and $\mathsf{n} = 10$, the error first decreases as $\mathcal{O}(\Delta^2)$ for large time step size and then as $\mathcal{O}(\Delta)$ for small time step size; see Table 6. When $\mathsf{N} = 2$ and $\mathsf{n} = 10$, the errors with $\Delta = 0.005, 0.002, 0.001$ are 10% $(1/\mathsf{n})$ of those with the same parameters but $\mathsf{n} = 1$ in Table 5. Here the constant in front of Δ, C/n, plays an important

Table 6

Algorithm 2.1*: recursive multistage WCE for* (4.7) *at* $T = 1$*:* $\sigma_1 = 0.5$*,* $\sigma_2 = 0.2$*,* $\beta = 0.1$*,* $\epsilon = 0.02$*. The parameters are* $\mathsf{M} = 20$*,* $\mathsf{N} = 2$*, and* $\mathsf{n} = 10$*. The time step size* δt *is* $\Delta/10$*.*

Δ	$\bar{\varrho}_2^{r,2}(T)$	Order	$\bar{\varrho}_2^{r,\infty}(T)$	Order	CPU time (sec.)
1.0e-1	4.9310e-05	–	2.6723e-05	–	84.00
5.0e-2	1.4031e-05	$\Delta^{1.81}$	7.3571e-06	$\Delta^{1.86}$	160.50
2.0e-2	2.9085e-06	$\Delta^{1.71}$	1.4171e-06	$\Delta^{1.80}$	391.40
1.0e-2	9.8015e-07	$\Delta^{1.57}$	4.4324e-07	$\Delta^{1.68}$	749.40
5.0e-3	3.5978e-07	$\Delta^{1.45}$	1.5082e-07	$\Delta^{1.56}$	1557.60
2.0e-3	9.8910e-08	$\Delta^{1.41}$	3.8369e-08	$\Delta^{1.49}$	3887.50

role: when Δ is large and this constant is small, then the order of two can be observed; when Δ is small, $C\Delta/\mathsf{n}$ is dominant so that only first-order convergence can be observed.

The recursive multistage SCM is of first-order convergence when $\mathsf{L} = 2, 3, 4$ and $\mathsf{n} = 1, 2, 10$ (only parts of the results presented). In contrast to Example 4.2, the errors from $\mathsf{L} = 3$ are one order of magnitude smaller those from $\mathsf{L} = 2$. Recalling that the number of sparse grid points is $\eta(2, 2) = 5$ and $\eta(3, 2) = 13$, we have the cost for $\mathsf{L} = 3$ is about 2.6 times of that for $\mathsf{L} = 2$. However, it is expected that in practice, a low-level sparse grid is more efficient than a high-level one when $\mathsf{n}q$ is large as the number of sparse grid points $\eta(\mathsf{L}, \mathsf{n}q)$ is increasing exponentially with $\mathsf{n}q$ and L. In other words, $\mathsf{L} = 2$ is preferred when SPDEs with many noises (large q) are considered.

As discussed in the beginning of this section, the ratio of time cost for SCM and WCE is $\eta(\mathsf{L}, \mathsf{n}q)/\binom{\mathsf{N}+\mathsf{n}q}{\mathsf{N}}$. The cost of recursive multistage SCM with $\mathsf{L} = 2$ is at most 1.8 times (1.6 predicted by the ratio above, $q = 2$ and $\mathsf{n} = 1$) of that of recursive multistage WCE with $\mathsf{N} = 1$. However, in this example, the accuracy of the recursive multistage SCM is one order of magnitude smaller than that of the recursive multistage WCE when $\mathsf{N} = 1$ and $\mathsf{L} = 2$. In Table 5, we present in bold the errors between 3.5×10^{-5} and 8.0×10^{-5}. Among the four cases listed in the table, the most efficient, for the given accuracy above, is WCE with $\mathsf{N} = 2$, which outperforms SCM with $\mathsf{L} = 3$ and $\mathsf{L} = 2$. WCE with $\mathsf{N} = 1$ is less efficient than the other three cases. We also observed that when $\sigma_1 = \sigma_2 = 1$, SCM with $\mathsf{L} = 2$ is one order of magnitude smaller than WCE with $\mathsf{N} = 1$ (results not presented here).

For noncommutative noises in this example, we show that the error for WCE is $\Delta^2 + C\Delta/\mathsf{n}$ and the error for SCM is Δ. The numerical results suggest that SCM with $\mathsf{L} = 2$ is competitive with WCE with $\mathsf{N} = 1$ for both small and large magnitude of noises if $\mathsf{n} = 1$.

With these three examples, we observe that the convergence order of the recursive multistage SCM in the second-order moments is one for commutative and noncommutative noises. We verified that our error estimate for WCE, $\Delta^{\mathsf{N}} + \Delta^2$, is valid for commutative noises (see Examples 4.1 and 4.2); the numerical results for noncommutative noises (see Example 4.3) suggest the errors are of order $\Delta^{\mathsf{N}} + C\Delta/\mathsf{n}$, where C is a constant depending on the coefficients of the noises.

For stochastic advection-diffusion-reaction equations, different formulations of stochastic products (Ito–Wick product for WCE, Stratonovich product for SCM) lead to different numerical performances. When the white noise is in the velocity, the Ito formulation will have stronger diffusion than that in the Stratonovich formulation in the resulting PDE. As stronger diffusion requires more resolution, the recursive multistage WCE with $\mathsf{N} = 1$ may produce less accurate results than those by the recursive multistage SCM with $\mathsf{L} = 2$ with the same PDE solver under the same resolution, as shown in the first and third examples.

To achieve convergence of approximations of second moments with first order in time step Δ, we can use the recursive multistage SCM Algorithm 2.2 with $\mathsf{L} = 2$, $\mathsf{n} = 1$, and also the recursive multistage WCE Algorithm 2.1 with $\mathsf{N} = 1$, $\mathsf{n} = 1$, as both can outperform each other in certain cases. For commutative noises, Algorithm 2.1 with $\mathsf{N} = 2$ is preferable when the number of noises, q, is small and hence the number of WCE modes is small so that the computational cost would grow slowly.

We also note that the errors of Algorithms 2.1 and 2.2 depend on the SPDE coefficients and integration time (cf. theoretical results of section 3). For some SPDEs, the constants at powers of Δ in the errors can be very large and, to reach desired levels of accuracy, we need to use very small step size Δ or develop numerical algorithms further (e.g., higher-order or structure-preserving approximations; see such ideas for stochastic ordinary differential equations, e.g., in [26]). Further, in practice, we need to aim at balancing the three parts (truncation of Wiener processes, functional truncation of WCE/SCM, and space-time discretizations of the deterministic PDEs appearing in the algorithms) of the errors of Algorithms 2.1 and 2.2 for higher computational efficiency.

5. Proofs.

5.1. Proof of Theorem 3.1. The idea of the proof is to first establish an estimate for the one-step ($\Delta = T$) error where the global error can readily derived from. We need the following two lemmas for the one-step errors. Introduce (cf. (2.6))

$$u_{\mathsf{N}}(t,x) = \sum_{|\alpha| \leq \mathsf{N},\, \alpha \in \mathcal{J}_q} \frac{1}{\sqrt{\alpha!}} \varphi_\alpha(t,x) \xi_\alpha. \tag{5.1}$$

LEMMA 5.1. *Let $q = 1$ in (2.1). Assume that $\sigma_{i,1}, a_{i,j}, b_i, c, \nu_1$ belong to $\mathcal{C}_b^{r+1}(\mathcal{D})$ and $u_0 \in H^r(\mathcal{D})$, where $r \geq \mathsf{N} + 1$. Let u in (2.6) be the solution to (2.1) and u_{N} is from (5.1). For $C_1 < \delta_{\mathcal{L}}$, the following estimate holds:*

$$\begin{aligned} \mathbb{E}[\|u(\Delta,\cdot) - u_{\mathsf{N}}(\Delta,\cdot)\|^2] &\leq (C_{\lfloor r \rfloor}\Delta)^{\mathsf{N}+1} e^{2C_{\mathcal{L}}\Delta} \\ &\times \left[\frac{e^{C_{\lfloor r \rfloor}\Delta}}{(\mathsf{N}+1)!} + \frac{(C_{\lfloor r \rfloor}\Delta)^{\lfloor r \rfloor - \mathsf{N} - 1}}{\lfloor r \rfloor !} \frac{\delta_{\mathcal{L}}}{\delta_{\mathcal{L}} - C_1} \right] \|u_0\|^2_{H^{\lfloor r \rfloor}}, \end{aligned}$$

where the constants $\delta_{\mathcal{L}}$ and $C_{\mathcal{L}}$ are from (2.3) and $C_{\lfloor r \rfloor}$ is from (3.5).

LEMMA 5.2. *Under the assumptions of Lemma 5.1 and $r \geq \mathsf{N} + 2$, we have*

$$\mathbb{E}[\|u_{\mathsf{N},\mathsf{n}}(\Delta,\cdot) - u_{\mathsf{N}}(\Delta,\cdot)\|^2] \leq \frac{2\Delta^3}{\mathsf{n}\pi^2} C(\mathsf{N}+2,\mathcal{L}) \tilde{C}(\mathsf{N},\mathcal{L}) C_{\mathsf{N}+2} e^{2C_{\mathsf{N}+2}\Delta + 2C_{\mathcal{L}}\Delta} \|u_0\|^2_{H^{\mathsf{N}+2}},$$

where $C_{\mathcal{L}}$ is from (2.3), $C(\mathsf{N}+2,\mathcal{L})$ is from (3.1), $\tilde{C}(\mathsf{N},\mathcal{L})$ is from (3.4), and $C_{\mathsf{N}+2}$ is from (3.5).

Using Lemmas 5.1 and 5.2, we can establish the estimate of the global error stated in Theorem 3.1. Specifically, the one-step error is bounded by the sum of $\mathbb{E}[(u(\Delta) - u_{\mathsf{N}}(\Delta))^2]$ and $\mathbb{E}[(u_{\mathsf{N}}(\Delta) - u_{\mathsf{N},\mathsf{n}}(\Delta))^2]$, which are estimated in Lemmas 5.1 and 5.2. Then, the global error is estimated based on the recursion nature of Algorithm 2.1 as in the proof in [21, Theorem 2.4], which completes the proof of Theorem 3.1.

Now we proceed to proving Lemmas 5.1 and 5.2. Let us denote by $\mathbf{s}^k$ the ordered set $(s_1, \ldots, s_k)$, and for $k \geq 1$, denote $d\mathbf{s}^k := ds_1 \ldots ds_k$, and

$$\int^{(k)} (\cdots)\, d\mathbf{s}^k = \int_0^{\Delta} \int_0^{s_k} \cdots \int_0^{s_2} (\cdots)\, ds_1 \ldots ds_k,$$
$$\int_{(k)} (\cdots)\, d\mathbf{s}^k = \int_0^{\Delta} \int_{s_1}^{\Delta} \cdots \int_{s_{k-1}}^{\Delta} (\cdots)\, ds_k \ldots ds_2\, ds_1,$$

and $F(\Delta; \mathbf{s}^k; x) = \mathcal{T}_{\Delta - s_k} \mathcal{M} \cdots \mathcal{T}_{s_2 - s_1} \mathcal{M} \mathcal{T}_{s_1} u_0(x)$, where $\mathcal{M} := \mathcal{M}_1$.

Proof of Lemma 5.1. It follows from (2.3) and the assumptions on the coefficients that (3.1) and (3.2) hold; cf. [11, section 7.1.3]. Also, by the assumption that $\sigma_{i,1}, \nu_1$ belong to $\mathcal{C}_b^{r+1}(\mathcal{D})$, it can be readily checked that (3.3) holds.

By (2.6), (5.1) and orthogonality of ξ_α (see (2.7)), we have

$$\mathbb{E}[\left\| u(\Delta, \cdot) - u_{\mathsf{N}}(\Delta, \cdot) \right\|^2] = \sum_{k > N} \sum_{|\alpha| = k} \frac{\left\| \varphi_\alpha(\Delta, \cdot) \right\|^2}{\alpha!}.$$

Similar to the proof of Proposition A.1 in [21], we have

$$\sum_{|\alpha|=k} \frac{\varphi_\alpha^2(\Delta, x)}{\alpha!} = \int^{(k)} \left| F(\Delta; \mathbf{s}^k; x) \right|^2 \, d\mathbf{s}^k.$$

Then by the Fubini theorem,

$$\sum_{|\alpha|=k} \frac{\left\| \varphi_\alpha(\Delta, \cdot) \right\|^2}{\alpha!} = \int^{(k)} \left\| F(\Delta; \mathbf{s}^k; \cdot) \right\|^2 d\mathbf{s}^k. \tag{5.2}$$

Assume that $r > 0$ is an integer. When $r > 0$ is not an integer, we use $\lfloor r \rfloor$ instead.

Denote $X_k = \mathcal{T}_{s_k - s_{k-1}} \mathcal{M} \cdots \mathcal{T}_{s_2 - s_1} \mathcal{M} \mathcal{T}_{s_1} u_0$, $Y_k = \mathcal{M} X_k$, $k \geq 1$, and also $X = \mathcal{T}_{\Delta - s_k} Y_k$. Then $X_k = \mathcal{T}_{s_k - s_{k-1}} Y_{k-1}$ and $Y_{k-1} = \mathcal{M} X_{k-1}$.

By the definition of F, (3.1), (3.3), and (3.5), we have for $r \geq k$

$$\begin{aligned}
\left\| F(\Delta; \mathbf{s}^k; \cdot) \right\|^2 &\leq e^{2C_{\mathcal{L}}(\Delta - s_k)} \left\| Y_k \right\|_{H^0}^2 = e^{2C_{\mathcal{L}}(\Delta - s_k)} \left\| \mathcal{M}_{i_k} X_k \right\|_{H^0}^2 \\
&\leq \tilde{C}(0, \mathcal{M}) e^{2C_{\mathcal{L}}(\Delta - s_k)} \left\| X_k \right\|_{H^1}^2 \\
&\leq C_1 e^{2C_{\mathcal{L}}(\Delta - s_{k-1})} \left\| Y_{k-1} \right\|_{H^1}^2 \leq \cdots \leq C_k^k e^{2C_{\mathcal{L}}\Delta} \left\| u_0 \right\|_{H^k}^2,
\end{aligned}$$

where $\tilde{C}(r-1, \mathcal{M})$ is from (3.3) and C_k is defined in (3.5). We then have

$$\int^{(k)} \left\| F(\Delta; \mathbf{s}^k; \cdot) \right\|^2 d\mathbf{s}^k \leq C_k^k e^{2C_{\mathcal{L}}\Delta} \left\| u_0 \right\|_{H^k}^2 \int^{(k)} d\mathbf{s}^k. \tag{5.3}$$

If $r < k$, by changing the integration order and applying (3.1), (3.3), and (3.2), we get

$$\begin{aligned}
\int^{(k)} \left\|F(\Delta; \mathbf{s}^k; \cdot)\right\|^2 d\mathbf{s}^k &= \int^{(k)} \left\|X\right\|^2 d\mathbf{s}^k = \int_{(k)} \left\|X\right\|^2 d\mathbf{s}^k \\
&\le \int_{(k)} e^{2C_{\mathcal{L}}(\Delta - s_k)} \left\|Y_k\right\|^2 d\mathbf{s}^k = \int_{(k)} e^{2C_{\mathcal{L}}(\Delta - s_k)} \left\|\mathcal{M}_{i_k} X_k\right\|^2 d\mathbf{s}^k \\
&\le \tilde{C}(0, \mathcal{M}) \int_{(k)} e^{2C_{\mathcal{L}}(\Delta - s_k)} \left\|X_k\right\|^2_{H^1} d\mathbf{s}^k \\
&= \tilde{C}(0, \mathcal{M}) \int_{(k-1)} \int_{s_{k-1}}^{\Delta} e^{2C_{\mathcal{L}}(\Delta - s_k)} \left\|X_k\right\|^2_{H^1} ds_k \, d\mathbf{s}^{k-1} \\
&\le \delta_{\mathcal{L}}^{-1} C_1 \int_{(k-1)} e^{2C_{\mathcal{L}}(\Delta - s_{k-1})} \left\|Y_{k-1}\right\|^2 d\mathbf{s}^{k-1},
\end{aligned}$$

where C_1 is from (3.5). Repeating this procedure and using (5.3), we obtain

$$\begin{aligned}
\int^{(k)} \left\|F(t; s^k; \cdot)\right\|^2 d\mathbf{s}^k &\le \delta_{\mathcal{L}}^{r-k} C_1^{k-r} \int_{(r)} e^{2C_{\mathcal{L}}(\Delta - s_r)} \left\|Y_r\right\|^2 ds^r \\
&\le \delta_{\mathcal{L}}^{r-k} C_1^{k-r} C_r^r e^{2C_{\mathcal{L}} t} \left\|u_0\right\|^2_{H^r} \int^{(r)} d\mathbf{s}^r. \qquad (5.4)
\end{aligned}$$

By (5.1), (5.2), (5.3), and (5.4), and $\int^{(k)} d\mathbf{s}^k = \frac{\Delta^k}{k!}$, we conclude that, for $r \ge \mathsf{N}+1$ and $C_1 < \delta_{\mathcal{L}}$,

$$\begin{aligned}
\mathbb{E}[\left\|u(\Delta, \cdot) - u_{\mathsf{N}}(\Delta, \cdot)\right\|^2] &= \sum_{\mathsf{N} < k \le r} \int^{(k)} \left\|F(\Delta; \mathbf{s}^k; \cdot)\right\|^2 d\mathbf{s}^k + \sum_{k > r} \int^{(k)} \left\|F(\Delta; \mathbf{s}^k; \cdot)\right\|^2 d\mathbf{s}^k \\
&\le \sum_{\mathsf{N} < k \le r} \frac{\Delta^k}{k!} C_r^k e^{2C_{\mathcal{L}}\Delta} \left\|u_0\right\|^2_{H^k} + \frac{\Delta^r}{r!} C_r^r e^{2C_{\mathcal{L}}\Delta} \left\|u_0\right\|^2_{H^r} \sum_{k > r} \delta_{\mathcal{L}}^{r-k} C_1^{k-r} \\
&\le (C_r \Delta)^{\mathsf{N}+1} e^{2C_{\mathcal{L}}\Delta} \left[\frac{e^{C_r \Delta}}{(\mathsf{N}+1)!} + \frac{(C_r\Delta)^{r-\mathsf{N}-1}}{r!} \frac{\delta_{\mathcal{L}}}{\delta_{\mathcal{L}} - C_1} \right] \left\|u_0\right\|^2_{H^r}. \qquad \square
\end{aligned}$$

Remark 5.1. Lemma 5.1 holds for $r = \infty$ if $C_\infty < \infty$. Based on (5.3), we can prove that

$$\begin{aligned}
\mathbb{E}[\left\|u(\Delta, \cdot) - u_{\mathsf{N}}(\Delta, \cdot)\right\|^2] &\le \sum_{k \ge \mathsf{N}} \frac{\Delta^k}{k!} C_\infty^k e^{2C_{\mathcal{L}}\Delta} \left\|u_0\right\|^2_{H^k} \\
&\le (C_\infty \Delta)^{\mathsf{N}+1} e^{2C_{\mathcal{L}}\Delta} \frac{e^{C_\infty \Delta}}{(\mathsf{N}+1)!} \left\|u_0\right\|^2_{H^\infty}.
\end{aligned}$$

If $r < \infty$, we need to require that $C_1 < \delta_{\mathcal{L}}$, i.e., $\tilde{C}(0, \mathcal{M}) C(1, \mathcal{L}) < \delta_{\mathcal{L}}$. For example, $\mathcal{L} = \triangle$, $\mathcal{M}_1 = \frac{1}{2} D_1$, for which $\tilde{C}(0, \mathcal{M}) C(1, \mathcal{L}) = \frac{1}{2} < \delta_{\mathcal{L}} = 1$.

Proof of Lemma 5.2. It can be proved as in [21, p. 447] that

$$\mathbb{E}[|u_{\mathsf{N}}(\Delta, \cdot) - u_{\mathsf{N},\mathsf{n}}(\Delta, \cdot)|^2] = \sum_{l \ge \mathsf{n}+1} \sum_{k=1}^{\mathsf{N}} \sum_{|\alpha| = k, i_k^\alpha = l} \frac{\varphi_\alpha^2(\Delta, \cdot)}{\alpha!}, \qquad (5.5)$$

where $i^\alpha_{|\alpha|}$ is the index of the last nonzero element of α and the last summation in the right-hand side can be bounded by (see [21, (3.7)])

$$\sum_{|\alpha|=k,i^\alpha_k=l} \frac{\varphi^2_\alpha(\Delta,x)}{\alpha!} \le \int^{(k-1)} \left| \sum_{j=1}^k \int_{s_{j-1}}^{s_{j+1}} F_j(\Delta;\mathbf{s}^k;x) M_l(s_j)\, ds_j \right|^2 d\mathbf{s}^k_j,$$

where $d\mathbf{s}^k_j = ds_1 \cdots ds_{j-1}\, ds_{j+1} \cdots ds_k$, $s_0 := 0$, $s_{k+1} := \Delta$, $M_l(t) = \int_0^t m_l(s)\, ds$, and

$$\begin{aligned} F_j(\Delta;\mathbf{s}^k;x) = \frac{\partial F(\Delta;\mathbf{s}^k;x)}{\partial s_j} &= \mathcal{T}_{\Delta-s_k}\mathcal{M}\cdots\mathcal{T}_{s_{j+1}-s_j}\mathcal{M}\mathcal{L}\mathcal{T}_{s_j-s_{j-1}}\cdots\mathcal{T}_{s_1}u_0(x) \\ &\quad - \mathcal{T}_{\Delta-s_k}\mathcal{M}\cdots\mathcal{M}\mathcal{L}\mathcal{T}_{s_{j+1}-s_j}\cdots T_{s_1}u_0(x) =: F^1_j + F^2_j. \end{aligned}$$

Then by the Fubini theorem and the Cauchy–Schwarz inequality, we have

$$\sum_{|\alpha|=k,i^\alpha_k=l} \frac{\left\|\varphi_\alpha(\Delta,\cdot)\right\|^2}{\alpha!} \le k \int^{(k-1)} \sum_{j=1}^k \int_{s_{j-1}}^{s_{j+1}} \left\|F_j(\Delta;\mathbf{s}^k;\cdot)\right\|^2 ds_j \int_{s_{j-1}}^{s_{j+1}} M^2_l(s_j)\, ds_j\, d\mathbf{s}^k_j.$$

We claim (see its proof below) that

$$\left\|F_j(\Delta;\mathbf{s}^k;\cdot)\right\|^2 \le 2 \max_{1\le j\le k} \left\|F^1_j\right\|^2 \le 2C^k_{k+2}\tilde{C}(k,\mathcal{L})C(k+2,\mathcal{L})e^{2C_\mathcal{L}\Delta}\left\|u_0\right\|^2_{H^{k+2}}. \tag{5.6}$$

Thus, by (5.6) we have

$$\sum_{|\alpha|=k,i^\alpha_k=l} \frac{\left\|\varphi_\alpha(\Delta,\cdot)\right\|^2}{\alpha!} \le 2k\Delta C^k_{k+2}C(k+2,\mathcal{L})\tilde{C}(k,\mathcal{L})e^{2C_\mathcal{L}\Delta}\left\|u_0\right\|^2_{H^{k+2}} \int_0^\Delta M^2_l(s)\, ds \int^{(k-1)} d\mathbf{s}^k_j. \tag{5.7}$$

Then by (5.5), (5.7), and $M_l(t) = \frac{\sqrt{2\Delta}}{(l-1)\pi}\sin(\frac{(l-1)\pi}{\Delta}t)$ (by (2.12)), we obtain that

$$\begin{aligned} \mathbb{E}[\left\|u_\mathsf{N}(\Delta,\cdot) - u_{\mathsf{N},\mathsf{n}}(\Delta,\cdot)\right\|^2] &\le \sum_{l\ge \mathsf{n}+1} \frac{\Delta^2}{(l-1)^2\pi^2} e^{2C_\mathcal{L}\Delta} \\ &\quad \times \sum_{k=1}^{\mathsf{N}} C^k_{k+2}C(k+2,\mathcal{L})\tilde{C}(k,\mathcal{L})\left\|u_0\right\|^2_{H^{k+2}} \frac{2k\Delta^k}{(k-1)!} \\ &\le \frac{2\Delta^3}{\mathsf{n}\pi^2} e^{2C_\mathcal{L}\Delta} \sum_{k=1}^{\mathsf{N}} C^k_{k+2}\tilde{C}(k,\mathcal{L})C(k+2,\mathcal{L})\left\|u_0\right\|^2_{H^{k+2}} \frac{k\Delta^{k-1}}{(k-1)!} \\ &\le \frac{2\Delta^3}{\mathsf{n}\pi^2} C_{\mathsf{N}+2}C(\mathsf{N}+2,\mathcal{L})\tilde{C}(\mathsf{N},\mathcal{L})e^{2C_{\mathsf{N}+2}\Delta+2C_\mathcal{L}\Delta}\left\|u_0\right\|^2_{H^{\mathsf{N}+2}}. \end{aligned}$$

It remains to prove (5.6). Note that it is sufficient to estimate $\left\|F^1_j\right\|$ due to the same structure of the two terms in $F_j(\Delta;\mathbf{s}^k;x)$. By the assumption that $a_{i,j}$ b_i

and c belongs to $\mathcal{C}_b^{\mathsf{N}+3}(\mathcal{D})$, it can be readily checked that (3.4) holds with $l \le \mathsf{N}+1$. Repeatedly using (3.1) and (3.3) gives

$$\begin{aligned}
\left\|F_j^1\right\|^2 &= \left\|\mathcal{T}_{\Delta-s_k}\mathcal{M}\cdots\mathcal{T}_{s_{j+1}-s_j}\mathcal{M}\mathcal{L}\mathcal{T}_{s_j-s_{j-1}}\cdots\mathcal{T}_{s_1}u_0\right\|^2\\
&\le e^{2C_{\mathcal{L}}(\Delta-s_k)}\left\|\mathcal{M}\cdots\mathcal{T}_{s_{j+1}-s_j}\mathcal{M}\mathcal{L}\mathcal{T}_{s_j-s_{j-1}}\cdots\mathcal{T}_{s_1}u_0\right\|^2\\
&\le \tilde{C}(0,\mathcal{M})e^{2C_{\mathcal{L}}(\Delta-s_k)}\left\|\mathcal{T}_{s_k-s_{k-1}}\cdots\mathcal{T}_{s_{j+1}-s_j}\mathcal{M}\mathcal{L}\mathcal{T}_{s_j-s_{j-1}}\cdots\mathcal{T}_{s_1}u_0\right\|_{H^1}^2\\
&\le C_1e^{2C_{\mathcal{L}}(\Delta-s_{k-1})}\left\|\mathcal{M}\cdots\mathcal{T}_{s_{j+1}-s_j}\mathcal{M}\mathcal{L}\mathcal{T}_{s_j-s_{j-1}}\cdots\mathcal{T}_{s_1}u_0\right\|_{H^1}^2\\
&\le\cdots\le C_{k-j}^{k-j}e^{2C_{\mathcal{L}}(\Delta-s_j)}\left\|\mathcal{M}\mathcal{L}\mathcal{T}_{s_j-s_{j-1}}\cdots\mathcal{T}_{s_1}u_0\right\|_{H^{k-j}}^2\\
&\le C_{k-j}^{k-j}\tilde{C}(k-j,\mathcal{M})e^{2C_{\mathcal{L}}(\Delta-s_j)}\left\|\mathcal{L}\mathcal{T}_{s_j-s_{j-1}}\cdots\mathcal{T}_{s_1}u_0\right\|_{H^{k-j+1}}^2\\
&\le C_{k-j}^{k-j}\tilde{C}(k-j,\mathcal{M})\tilde{C}(k-j+1,\mathcal{L})e^{2C_{\mathcal{L}}(\Delta-s_j)}\left\|\mathcal{T}_{s_j-s_{j-1}}\cdots\mathcal{T}_{s_1}u_0\right\|_{H^{k-j+3}}^2\\
&\le C_{k-j+1}^{k-j+1}\tilde{C}(k-j+1,\mathcal{L})e^{2C_{\mathcal{L}}(\Delta-s_j)}\left\|\mathcal{T}_{s_j-s_{j-1}}\mathcal{M}\cdots\mathcal{T}_{s_1}u_0\right\|_{H^{k-j+3}}^2,
\end{aligned}$$

where we have used (3.4) in the next-to-last line and the fact that $C(k-j+1,\mathcal{L})\ge 1$. Similarly, we have

$$\left\|\mathcal{T}_{s_j-s_{j-1}}\mathcal{M}\cdots\mathcal{T}_{s_1}u_0\right\|_{H^{k-j+3}}^2 \le C(k-j+3,\mathcal{L})C_{k+2}^{j-1}e^{2C_{\mathcal{L}}s_j}\left\|u_0\right\|_{H^{k+2}}^2.$$

Thus, we arrive at (5.6). This ends the proof of Lemma 5.2. $\square$

5.2. Proof of Theorem 3.3. To prove Theorem 3.3, we need a probabilistic representation of the solution to (2.1). Let $(\{B_k(s)\}, 1\le k\le d, \mathcal{F}_s^B)$ be a system of one-dimensional standard Wiener processes on a complete probability space $(\Omega^1,\mathcal{F}^1,Q)$ and independent of $w(s)$ on the space $(\Omega\otimes\Omega^1,\mathcal{F}\otimes\mathcal{F}^1,P\otimes Q)$. Consider the following backward stochastic differential equation on $(\Omega^1,\mathcal{F}^1,Q)$ for $0\le s\le t$:

$$\hat{d}\hat{X}_{t,x}(s) = b(\hat{X}_{t,x}(s))\,ds + \sum_{r=1}^{d}\alpha_r(\hat{X}_{t,x}(s))\,\hat{d}B_r(s),\quad \hat{X}_{t,x}(t)=x. \tag{5.8}$$

The symbol "$\hat{d}$" means backward integral; see, e.g., [19, 30] for treatment of backward stochastic integrals. The $d\times d$ matrix $\alpha(x)$ is defined by $\alpha(x)\alpha^{\mathsf{T}}(x)=2a(x)$. Here $a(x)$ and $b(x)$ are from (2.2). Consider the following backward stochastic differential equation on $(\Omega\otimes\Omega^1,\mathcal{F}\otimes\mathcal{F}^1,P\otimes Q)$ for $0\le s\le t$:

$$\hat{d}\hat{Y}_{t,1,x}(s) = c(\hat{X}_{t,x}(s))\hat{Y}_{t,1,x}(s)\,ds + \textstyle\sum_{r=1}^{q}\nu_r(\hat{X}_{t,x}(s))\hat{Y}_{t,1,x}(s)]\,\hat{d}w_r,\quad \hat{Y}_{t,1,x}(t)=1. \tag{5.9}$$

Here $c(x)$ and $\nu_r(x)$ are from (2.2). When $u_0(x)\in\mathcal{C}_b^2(\mathcal{D})$ and $\alpha(x)$, $b(x)$, $c(x)$, $\nu_r(x)\in\mathcal{C}_b^0(\mathcal{D})$ and $\sigma_{i,r}=0$, the solution to (2.1)–(2.2) can be represented by (see e.g., [19])

(5.10)
$$u(t,x)=\mathbb{E}_Q\left[u_0(\hat{X}_{t,x}(0))\exp\left(\sum_{r=1}^{q}\int_0^t\nu_r(\hat{X}_{t,x}(s))\,\hat{d}w_r(s)+\int_0^t\bar{c}(\hat{X}_{t,x}(s))\,ds\right)\right],$$

where $\bar{c}(x)=c(x)-\frac{1}{2}\sum_{r=1}^{q}\nu_r^2(x)$.

Here we first establish the one-step error (3.9) and then the global error (3.10) We follow the recipe of the proofs in [16, Theorem 3.1] and [5, Theorem 4.4], where $\mathsf{n}=1$ and $\mathsf{K}>1$.

We need the following mean-square convergence rate for the one-step error.

Proposition 5.3 (mean-square convergence). *Assume that $\sigma_{i,r} = 0$ and that the initial condition u_0 and the coefficients in (2.2) are in $\mathcal{C}_b^2(\mathcal{D})$. Let $u(t,x)$ be the solution to (2.1) and $\tilde{u}_{\Delta,\mathsf{n}}(t,x)$ the solution to (2.16). Then for any $\varepsilon > 0$,*

$$\mathbb{E}[|u(\Delta,x) - \tilde{u}_{\Delta,\mathsf{n}}(\Delta,x)|^2] \le C\exp(C\Delta)(\Delta^3 + \Delta^2)\mathsf{n}^{-1+\varepsilon}, \tag{5.11}$$

where the constant $C > 0$ is independent of n.

Proof. The solution to (2.16) using the spectral truncation of Brownian motion $w_r^{(\Delta,\mathsf{n})}$ from (2.13) can be represented by (see, e.g., [5, 16])

$$\tilde{u}_{\Delta,\mathsf{n}}(\Delta,x) = \mathbb{E}_Q[u_0(\hat{X}_{\Delta,x}(0))\exp(\textstyle\sum_{r=1}^q \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s))\,dw_r^{(\Delta,\mathsf{n})}(s) + \int_0^\Delta \bar{c}(\hat{X}_{\Delta,x}(s))\,ds)]. \tag{5.12}$$

Using $e^x - e^y = e^{\theta x + (1-\theta)y}(x-y)$, $0 \le \theta \le 1$, boundedness of $\bar{c}(x)$ and $u_0(x)$, and the Cauchy–Schwarz inequality (twice), we have for some $C > 0$

$$\begin{aligned}
&\mathbb{E}[|\tilde{u}_{\Delta,\mathsf{n}}(\Delta,x) - u(\Delta,x)|^2] \\
&\quad = \mathbb{E}\Bigg[\Bigg(\mathbb{E}_Q\Bigg[u_0(\hat{X}_{\Delta,x}(0))\exp\left(\int_0^\Delta \bar{c}(\hat{X}_{\Delta,x}(s))\,ds\right) \\
&\qquad \times \exp\left(\sum_{r=1}^q \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s))[\theta\,dw_r^{(\Delta,\mathsf{n})}(s) + (1-\theta)\,\hat{d}w_r(s)]\right) \\
&\qquad \times \left(\sum_{r=1}^q \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s))[\,dw_r^{(\Delta,\mathsf{n})}(s) - \,\hat{d}w_r(s)]\right)\Bigg]\Bigg)^2\Bigg] \\
&\quad \le C\exp(C\Delta)\mathbb{E}\Bigg[\Bigg(\mathbb{E}_Q\Bigg[\exp\left(\sum_{r=1}^q \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s))[\theta\,dw_r^{(\Delta,\mathsf{n})}(s) + (1-\theta)\,\hat{d}w_r(s)]\right) \\
&\qquad \times \left|\sum_{r=1}^q \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s))[\,dw_r^{(\Delta,\mathsf{n})}(s) - \,\hat{d}w_r(s)]\right|\Bigg]\Bigg)^2\Bigg] \\
&\quad \le C\exp(C\Delta)\left(\mathbb{E}\left[\mathbb{E}_Q\left[\exp\left(\sum_{r=1}^q \int_0^\Delta 4\nu_r(\hat{X}_{\Delta,x}(s))[\theta\,dw_r^{(\Delta,\mathsf{n})}(s) + (1-\theta)\,\hat{d}w_r(s)]\right)\right]\right]\right)^{1/2} \\
&\qquad \times \left(\mathbb{E}\left[\mathbb{E}_Q\left[\left(\sum_{r=1}^q \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s))[\,dw_r^{(\Delta,\mathsf{n})}(s) - \,\hat{d}w_r(s)]\right)^4\right]\right]\right)^{1/2}.
\end{aligned} \tag{5.13}$$

Recall that $\mathbb{E}[\cdot] = \mathbb{E}_P[\cdot]$ is the expectation with respect to P only. Hence, we need to estimate $\mathrm{I}_1 = \left(\mathbb{E}[\mathbb{E}_Q[(\sum_{r=1}^q \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s))[\,dw_r^{(\Delta,\mathsf{n})}(s) - \,\hat{d}w_r(s)])^4]]\right)^{1/2}$ and

$$\mathrm{I}_2 = \left(\mathbb{E}\left[\left(\mathbb{E}_Q\left[\exp\left(\sum_{r=1}^q \int_0^\Delta 4\nu_r(\hat{X}_{\Delta,x}(s))[\theta\,dw_r^{(\Delta,\mathsf{n})}(s) + (1-\theta)\,\hat{d}w_r(s)]\right)\right]\right)\right]\right)^{1/2}.$$

We first estimate I_1. Due to the independence of B_k and w_r, and according to [28] and (2.5), we have

$$\int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s))\, \hat{d}w_r(s) = \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s)) \circ dw_r(s)$$
$$= \sum_{i=0}^{\infty} \xi_{r,i} \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s)) m_{r,i}(s)\, ds.$$

Thus by the Fubini theorem, (2.5), and (2.13), we can represent I_1 as

$$\mathrm{I}_1 = \left(\mathbb{E}_Q\left[\mathbb{E}\left[\left| \sum_{r=1}^{q} \left[\int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s))\, dw_r^{(\Delta,\mathsf{n})}(s) - \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s)) \circ dw_r(s) \right] \right|^4 \right] \right] \right)^{1/2}$$
$$= \left(\mathbb{E}_Q\left[\mathbb{E}\left[\left| \sum_{r=1}^{q} \sum_{i=\mathsf{n}+1}^{\infty} \xi_{r,i} \int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s)) m_{r,i}(s)\, ds \right|^4 \right] \right] \right)^{1/2}$$
$$\leq \left(3\mathbb{E}_Q\left[\left(\sum_{r=1}^{q} \sum_{i=\mathsf{n}+1}^{\infty} \left(\int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s)) m_{r,i}(s)\, ds \right)^2 \right)^2 \right] \right)^{1/2},$$

where we have used twice the fact that $\hat{X}_{\Delta,x}$ are independent of w_r and $w_r^{(\Delta,\mathsf{n})}$. Then by standard estimates of L^2-projection error (cf. [7, (5.1.10)]), we have for $0 < \varepsilon < 1$,

$$\text{(5.14)} \quad \sum_{i=\mathsf{n}+1}^{\infty} \left(\int_0^\Delta \nu_r(\hat{X}_{\Delta,x}(s)) m_{r,i}(s)\, ds \right)^2 \leq C\Delta^{1-\varepsilon} \mathsf{n}^{-1+\varepsilon} \left| \nu_r(\hat{X}_{\Delta,x}(\cdot)) \right|^2_{\frac{1-\varepsilon}{2},2,[0,\Delta]},$$

where the Slobodeckij seminorm $|f|_{\theta,p,[0,\Delta]}$ is defined by $(\int_0^\Delta, \int_0^\Delta \frac{|f(x)-f(y)|^p}{|x-y|^{p\theta+1}}\, dx\, dy)^{1/p}$ and the constant $\Delta^{1-\varepsilon}$ appears due to the length of domain; see, e.g., [7, Chapter 5.4]. Thus, we obtain

$$\text{(5.15)} \quad \mathrm{I}_1 \leq C\Delta^{1-\varepsilon} \mathsf{n}^{-1+\varepsilon} \left(\sum_{r=1}^{q} \mathbb{E}_Q\left[\left| \nu_r(\hat{X}_{\Delta,x}(\cdot)) \right|^4_{\frac{1-\varepsilon}{2},2,[0,\Delta]} \right] \right)^{1/2}, \ 0 < \varepsilon < 1.$$

By (5.8) and the Ito formula, we have

$$\hat{X}_{\Delta,x}(s) - \hat{X}_{\Delta,x}(s_1) = \int_{s_1}^{s} b(\hat{X}_{\Delta,x}(s_2))\, ds_2$$
$$+ \sum_{k=1}^{p} \alpha_k(\hat{X}_{\Delta,x}(s_1))[B_k(s) - B_k(s_1)] + R(s_1, s),$$

where $\mathbb{E}_Q[|R(s_1,s)|^{2l}] \leq C\,|s_1 - s|^{2l}$ $(l \geq 1)$ when $b(x)$ and $\alpha_k(x)$ belong to $\mathcal{C}_b^2(\mathcal{D})$. By the Lipschitz continuity of ν_1, the definition of the Slobodeckij seminorm, it is not difficult to show that

$$\text{(5.16)} \qquad \mathbb{E}_Q\left[\left| \nu_r(\hat{X}_{\Delta,x}(\cdot)) \right|^4_{\frac{1-\varepsilon}{2},2,[0,\Delta]} \right] \leq C(\Delta^{4+2\varepsilon} + \Delta^{2+2\varepsilon}).$$

Thus, by (5.15) and (5.16), we have

$$\mathrm{I}_1 \leq C(\Delta^3 + \Delta^2)\mathsf{n}^{-1+\varepsilon}. \tag{5.17}$$

Now we estimate I_2. Using the facts (see, e.g., [16, Lemma 2.5])

$$\mathbb{E}\left[\exp\left(\sum_{r=1}^{q}\int_0^\Delta 4\nu_r(\hat{X}_{\Delta,x}(s))\,dw_r\right)\right] = \exp\left(\sum_{r=1}^{q}8\int_0^\Delta \nu_r^2(\hat{X}_{\Delta,x}(s))\,ds\right),$$

$$\mathbb{E}\Bigg[\exp\left(\sum_{r=1}^{q}\int_0^\Delta 4\nu_r(\hat{X}_{\Delta,x}(s))\,dw_r^{(\Delta,\mathsf{n})}(s)\right)\Bigg] \leq 4\exp\left(\sum_{r=1}^{q}8\int_0^\Delta \nu_r^2(\hat{X}_{\Delta,x}(s))\,ds\right),$$

we have $\mathrm{I}_2 \leq 4\exp(C\Delta)$. From here, (5.17), and (5.13), we reach (5.11). ◻

Now we are ready to prove Theorem 3.3, i.e., the convergence in the second moments. For simplicity of notation, we consider $q = 1$, while the case $q > 1$ can be proved similarly. Denote

$$U_{\Delta,\mathsf{n},\mathsf{m},\theta}(t,x,\mathbf{y}) =: u_0(\hat{X}_{t,x}(0)) \times \exp\left(\sum_{i=1}^{\mathsf{n}}\nu_{1,i}y_i + \theta\sum_{j=\mathsf{n}+1}^{\mathsf{m}}\nu_{1,j}y_j + \int_0^t \bar{c}(\hat{X}_{t,x}(s))\,ds\right), \quad \mathsf{m} \geq \mathsf{n}.$$

where $\nu_{1,i}(t,x) = \int_0^t \nu_1(\hat{X}_{t,x}(s))m_i(s)\,ds$ for $i \leq \mathsf{m}$ ($\hat{X}_{t,x}(s)$ is the solution to (5.8)) and $\mathbf{y} = (y_1,\dots,y_\mathsf{n},y_{\mathsf{n}+1},\dots,y_\mathsf{m})$. Let us write $\tilde{u}_{\Delta,\mathsf{n},\mathsf{m},\theta}(t,x,\Xi) = \mathbb{E}_Q[U_{\Delta,\mathsf{n},\mathsf{m},\theta}(t,x,\Xi)]$, where $\Xi = (\xi_1,\dots,\xi_\mathsf{n},\xi_{\mathsf{n}+1},\dots,\xi_\mathsf{m})$. With this notation, we have

$$\tilde{u}_{\Delta,\mathsf{m}}(t,x) = \tilde{u}_{\Delta,\mathsf{n},\mathsf{m},1}(t,x,\Xi), \quad \tilde{u}_{\Delta,\mathsf{n}}(t,x) = \tilde{u}_{\Delta,\mathsf{n},\mathsf{m},0}(t,x,\Xi).$$

For $\mathsf{m} > \mathsf{n}$, by the first-order Taylor expansion, we have

$$\begin{aligned}
&\left|\mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{m}}(\Delta,x) - \tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x)]\right| \\
&\quad = \Bigg| 2\sum_{i,j=\mathsf{n}+1}^{\mathsf{m}}\frac{1}{(\delta_{i,j}+1)}\int_0^1 \theta(1-\theta) \\
&\qquad \times \mathbb{E}[\tilde{u}_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)\mathbb{E}_Q[U_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)\nu_{1,i}(t,x)\nu_{1,j}(t,x)]\xi_i\xi_j]\,d\theta \\
&\qquad + 2\sum_{i,j=\mathsf{n}+1}^{\mathsf{m}}\frac{1}{(\delta_{i,j}+1)}\int_0^1 \theta(1-\theta)\mathbb{E}[\mathbb{E}_Q[U_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)\nu_{1,i}(t,x)] \\
&\qquad \times \mathbb{E}_Q[U_{\Delta,\mathsf{n},\mathsf{m},\theta}(t,x,\Xi)\nu_{1,j}(t,x)]\xi_i\xi_j]\,d\theta \Bigg| \\
&\quad \leq 2\left|\int_0^1 (1-\theta)\theta\mathbb{E}\Bigg[\tilde{u}_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)\mathbb{E}_Q\Bigg[U_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\nu_{1,i}(\Delta,x)\xi_i\right)^2\Bigg]\Bigg]\,d\theta\right| \\
&\qquad + 2\left|\int_0^1 (1-\theta)\theta\mathbb{E}\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\mathbb{E}_Q\Big[U_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)\nu_{1,i}(\Delta,x)\Big]\xi_i\right)^2\right]\,d\theta\right|,
\end{aligned} \tag{5.18}$$

where $\delta_{i,j} = 1$ if $i = j$ and 0 otherwise and we have used the facts that ξ_i, $i > \mathsf{n}$, are independent of $\tilde{u}_\mathsf{n}(t,x)$ and $\mathbb{E}[\xi_i] = 0$.

By the Cauchy–Schwarz inequality (twice), we have for the first term in (5.18),

(5.19)
$$2\left|\int_0^1 (1-\theta)\theta\mathbb{E}\left[\tilde{u}_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)\mathbb{E}_Q\left[U_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\nu_{1,i}(\Delta,x)\xi_i\right)^2\right]\right]d\theta\right|$$
$$\leq C\left(\mathbb{E}\left[\mathbb{E}_Q\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\nu_{1,i}(\Delta,x)\xi_i\right)^8\right]\right]\right)^{1/4}.$$

Here we also used that $\mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)], \mathbb{E}[(\mathbb{E}_Q[U^2_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)])^2] \leq C$, which can be readily checked in the same way as in the proof of Proposition 5.3.

By the Taylor expansion for $U_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\mathbf{y})$, we have

$$U_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\mathbf{y}) = U_{\Delta,\mathsf{n},\mathsf{m},0}(\Delta,x,\mathbf{y})$$
$$+\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\nu_{1,i}(\Delta,x)\int_0^1(1-\theta_1)\theta_1\theta U_{\Delta,\mathsf{n},\mathsf{m},\theta\theta_1}(\Delta,x,\mathbf{y})\,d\theta_1 y_i.$$

Then by the Cauchy–Schwarz inequality (several times) and the fact that ξ_i, $i>\mathsf{n}$, are independent of $U_{\Delta,\mathsf{n},\mathsf{m},0}(t,x,\Xi)$, we have for the second term in (5.18),

(5.20)
$$2\left|\int_0^1(1-\theta)\theta\mathbb{E}\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\mathbb{E}_Q\left[U_{\Delta,\mathsf{n},\mathsf{m},\theta}(\Delta,x,\Xi)\nu_{1,i}(\Delta,x)\right]\xi_i\right)^2\right]d\theta\right|$$
$$\leq 4\left|\int_0^1(1-\theta)\theta\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\mathbb{E}\left[\left(\mathbb{E}_Q\left[U_{\Delta,\mathsf{n},\mathsf{m},0}(\Delta,x,\Xi)\nu_{1,i}(\Delta,x)\right]\right)^2\right]d\theta\right|$$
$$+4\left|\int_0^1(1-\theta)\theta^3\mathbb{E}\left[\left(\mathbb{E}_Q\left[\int_0^1(1-\theta_1)\theta_1U_{\Delta,\mathsf{n},\mathsf{m},\theta\theta_1}(\Delta,x,\Xi)\,d\theta_1\right.\right.\right.\right.$$
$$\left.\left.\left.\left.\times\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\nu_{1,i}(\Delta,x)\xi_i\right)^2\right]\right)^2\right]d\theta\right|$$
$$\leq\mathbb{E}[\mathbb{E}_Q[U^2_{\Delta,\mathsf{n},\mathsf{m},0}(\Delta,x,\Xi)]]\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\mathbb{E}_Q[\nu^2_{1,i}(\Delta,x)]$$
$$+C\left|\int_0^1(1-\theta)\theta^3\left(\mathbb{E}\left[\mathbb{E}_Q\left[\int_0^1(1-\theta_1)\theta_1U^4_{\Delta,\mathsf{n},\mathsf{m},\theta\theta_1}(\Delta,x,\Xi)\,d\theta_1\right]\right]\right)^{1/2}d\theta\right|$$
$$\times\left(\mathbb{E}\left[\mathbb{E}_Q\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\nu_{1,i}((\Delta,x)\xi_i)\right)^8\right]\right]\right)^{1/2}$$
$$\leq C\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\mathbb{E}_Q[\nu^2_{1,i}(\Delta,x)]+C\left(\mathbb{E}\left[\mathbb{E}_Q\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}}\nu_{1,i}(\Delta,x)\xi_i\right)^8\right]\right]\right)^{1/2}.$$

Here we used that $\mathbb{E}[\mathbb{E}_Q[U^2_{\Delta,\mathsf{n},\mathsf{m},,0}((\Delta,x,\Xi))]],\ \mathbb{E}[\mathbb{E}_Q[U^4_{\Delta,\mathsf{n},\mathsf{m},\theta\theta_1}(\Delta,x,\Xi)]] \le C$, which can be readily checked in the same way as in the proof of Proposition 5.3.

By (5.18), (5.19), and (5.20), we have

$$
\begin{aligned}
(5.21)\quad & \left|\mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{m}}(\Delta,x) - \tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x)]\right| \\
&\le C\sum_{i=\mathsf{n}+1}^{\mathsf{m}} \mathbb{E}_Q[\nu^2_{1,i}(\Delta,x)] + C\left(\mathbb{E}\left[\mathbb{E}_Q\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}} \nu_{1,i}(\Delta,x)\xi_i\right)^8\right]\right]\right)^{1/4} \\
&\quad + C\left(\mathbb{E}\left[\mathbb{E}_Q\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}} \nu_{1,i}(\Delta,x)\xi_i\right)^8\right]\right]\right)^{1/2}.
\end{aligned}
$$

Similar to the proof of (5.15), we have

$$
\begin{aligned}
\mathbb{E}\left[\mathbb{E}_Q\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}} \nu_{1,i}(\Delta,x)\xi_i\right)^8\right]\right] &\le C\mathbb{E}_Q\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}} \nu^2_{1,i}(\Delta,x)\right)^4\right] \\
&\le C\Delta^{4(1-\varepsilon)}\mathsf{n}^{4(1-\varepsilon)}\mathbb{E}_Q\left[\left|\nu_1(\hat{X}_{\Delta,x}(\cdot))\right|^8_{\frac{1-\varepsilon}{2},2,[0,\Delta]}\right].
\end{aligned}
$$

Similar to the proof of (5.16), we can estimate $\mathbb{E}_Q\left[\|\nu_1(\hat{X}_{\Delta,x}(\cdot))\|^8_{\frac{1-\varepsilon}{2},2,[0,\Delta]}\right]$ as follows:

$$
\mathbb{E}_Q\left[\left|\nu_1(\hat{X}_{\Delta,x}(\cdot))\right|^8_{\frac{1-\varepsilon}{2},2,[0,\Delta]}\right] \le C(\Delta^{8+4\varepsilon} + C\Delta^{4+4\varepsilon}),
$$

and thus

$$
(5.22)\qquad \mathbb{E}\left[\mathbb{E}_Q\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}} \nu_{1,i}(\Delta,x)\xi_i\right)^8\right]\right] \le C(\Delta^{12} + C\Delta^8).
$$

Similarly, we have

$$
(5.23)\quad \mathbb{E}\left[\mathbb{E}_Q\left[\left(\sum_{i=\mathsf{n}+1}^{\mathsf{m}} \nu_{1,i}(\Delta,x)\xi_i\right)^2\right]\right] = \sum_{i=\mathsf{n}+1}^{\mathsf{m}} \mathbb{E}_Q[\nu^2_{1,i}(\Delta,x)] \le C(\Delta^3 + C\Delta^2).
$$

By (5.21), (5.22), and (5.23), we have

$$
(5.24)\qquad \left|\mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{m}}(\Delta,x) - \tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x)]\right| \le C\exp(C\Delta)(\Delta^6 + \Delta^2)\mathsf{n}^{-1+\varepsilon}.
$$

By the triangle inequality and the Cauchy–Schwarz inequality, we obtain

$$
\begin{aligned}
\left|\mathbb{E}[u^2(\Delta,x) - \tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x)]\right| &\le \left|\mathbb{E}[u^2(\Delta,x) - \tilde{u}^2_{\Delta,\mathsf{m}}(\Delta,x)]\right| \\
&\quad + \left|\mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{m}}(\Delta,x) - \tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x)]\right|, \\
&\le C(\mathbb{E}[|u(\Delta,x) - \tilde{u}_{\Delta,\mathsf{m}}(\Delta,x)|^2])^{1/2} \\
&\quad + \left|\mathbb{E}[\tilde{u}^2_{\Delta,\mathsf{m}}(\Delta,x) - \tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x)]\right|.
\end{aligned}
$$

The one-step error (3.9) then follows from (5.24), Proposition 5.3, and taking m to $+\infty$. The global error (3.10) is estimated from the recursion nature of Algorithm 2.2 as in the proof in [21, Theorem 2.4]. $\square$

5.3. Proof of Theorem 3.4. For any n-dimensional function $\varphi(y_1, \ldots, y_\mathsf{n})$, we denote

$$I_\mathsf{n}\varphi = \frac{1}{(2\pi)^{\mathsf{n}/2}} \int_{\mathbb{R}^\mathsf{n}} \varphi(y_1, \ldots, y_\mathsf{n}) \exp\left(-\frac{1}{2}\sum_{i=1}^{\mathsf{n}} y_i^2\right) d\mathbf{y}.$$

Introduce the integrals

$$I_1^{(k)}\varphi = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \varphi(y_1, \ldots, y_k, \ldots, y_\mathsf{n}) \exp\left(-\frac{y_k^2}{2}\right) dy_k, \quad k = 1, \ldots, \mathsf{n}, \tag{5.25}$$

and their approximations $Q_n^{(k)}$ by the corresponding one-dimensional Gauss–Hermite quadratures with n nodes. Also, let $\mathcal{U}_{i_k}^{(k)} = Q_{i_k}^{(k)} - Q_{i_k-1}^{(k)}$. By the definition of Smolyak sparse grid and using the recipe from the proof of Lemma 3.4 in [27], we obtain

$$I_\mathsf{n}\varphi - A(\mathsf{L}, \mathsf{n})\varphi = \sum_{l=2}^{\mathsf{n}} S(\mathsf{L}, \mathsf{n}) \otimes_{k=l+1}^{\mathsf{n}} I_1^{(k)}\varphi + (I_1^{(1)} - Q_\mathsf{L}^{(1)}) \otimes_{k=2}^{\mathsf{n}} I_1^{(k)}\varphi, \tag{5.26}$$

where

$$S(\mathsf{L}, l) = \sum_{i_1+\cdots+i_{l-1}+i_l=\mathsf{L}+l-1} \otimes_{k=1}^{l-1}\mathcal{U}_{i_k}^{(k)} \otimes (I_1^{(l)} - Q_{i_l}^{(l)}). \tag{5.27}$$

Denote by D^α the multivariate derivatives with respect to $\mathbf{y}$. According to the proof of Proposition 3.1 in [38], we have

$$\begin{aligned}
&\left|S(\mathsf{L}, l) \otimes_{n=l+1}^{\mathsf{n}} I_1^{(n)}\varphi\right| \\
&\quad\le \sum_{i_1+\cdots+i_l=\mathsf{L}+l-1} \frac{(3c/2)^{\#G_{l-1}+1}}{(2\pi)^{(N-\#F_{l-1})/2}} \int_{\mathbb{R}^{\mathsf{n}-\#F_{l-1}}} \left|\otimes_{m\in F_{l-1}} Q_1^{(m)} D^{2\alpha_l}\varphi(\mathbf{y})\right| \\
&\quad\quad \times \exp\left(-\sum_{n\in G_{l-1}} \frac{\beta y_n^2}{2} - \frac{\beta y_l^2}{2} - \sum_{k=l+1}^{\mathsf{n}} \frac{y_k^2}{2}\right) \prod_{n\in G_{l-1}} dy_n \times dy_l \cdots dy_\mathsf{n},
\end{aligned} \tag{5.28}$$

where the multi-index $\alpha_l = (i_1 - 1, \ldots, i_{l-1} - 1, i_l, 0, \ldots, 0)$ with the mth element α_l^m, the sets $F_{l-1} = F_{l-1}(\alpha_l) = \{m : \ \alpha_l^m = 0, \ m = 1, \ldots, l-1\}$ and $G_{l-1} = G_{l-1}(\alpha_l) = \{m : \ \alpha_l^m > 0, \ m = 1, \ldots, l-1\}$, and the symbols $\#F_{l-1}$ and $\#G_{l-1}$ stand for the number of elements in the corresponding sets. Here $c > 0, \ 0 < \beta < 1$, are only related to the Gauss–Hermite quadrature, Q and are independent of the number of nodes in the Gauss–Hermite quadrature; see, e.g., [24, Theorem 2].

Proof of of Theorem 3.4. Setting $\varphi(y_1, \ldots, y_\mathsf{n}) = \tilde{u}_{\Delta,\mathsf{n}}^2(t, x, y_1, \ldots, y_\mathsf{n})$, we then have that $A(\mathsf{L}, \mathsf{n})\varphi$ is an approximation of the second moment of the solution obtained by the sparse grid collocation methods. Recall from (5.12) that $\tilde{u}_{\Delta,\mathsf{n}}(t, x, \mathbf{y}) = \mathbb{E}_Q[U_{\Delta,\mathsf{n}}(t, x, \mathbf{y})]$, where $U_{\Delta,\mathsf{n}}(t, x, \mathbf{y}) = U_{\Delta,\mathsf{n},\mathsf{m},0}(t, x, \mathbf{y})$.

Now we estimate $D^{2\alpha_l}[\tilde{u}_{\Delta,\mathsf{n}}^2(\Delta, x, y_1, \ldots, y_\mathsf{n})]$. To this end, we need to first estimate $D^{\beta_l}[\tilde{u}_{\Delta,\mathsf{n}}(\Delta, x, y_1, \ldots, y_\mathsf{n})]$, where $\beta_l \le 2\alpha_l$. By (5.14), we have for $0 < \varepsilon < 1$,

$$\nu_{1,k}^2(\Delta, x) \le C(\Delta \max(k-1, 1))^{\varepsilon-1} \left|\nu_1(\hat{X}_{\Delta,x}(\cdot))\right|^2_{\frac{1-\varepsilon}{2},2,[0,\Delta]},$$

and we have, by the Cauchy–Schwarz inequality,

$$
\begin{aligned}
(5.29)\qquad \left|D^{\beta_l}\tilde{u}_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})\right| &= \left|\mathbb{E}_Q\left[U_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})\prod_{k=1}^{l}(\nu_{1,k}(\Delta,x))^{\beta_l^k}\right]\right| \\
&\le \left(\mathbb{E}_Q\left[U^2_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})\right]\right)^{1/2}\left(\mathbb{E}_Q\left[\prod_{k=1}^{l}(\nu_{1,k}(\Delta,x))^{2\beta_l^k}\right]\right)^{1/2} \\
&\le (C\Delta^{1-\varepsilon})^{|\beta_l|/2}\prod_{k=2}^{l}(k-1)^{(\varepsilon-1)\beta_l^k/2}\left(\mathbb{E}_Q[U^2_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})]\right)^{1/2} \\
&\quad \times\left(\mathbb{E}_Q\left[\left|\nu_1(\hat{X}_{\Delta,x}(\cdot))\right|^{|2\beta_l|}_{\frac{1-\varepsilon}{2},2,[0,\Delta]}\right]\right)^{1/2}.
\end{aligned}
$$

By the chain rule for multivariate functions, we have

$$
D^{2\alpha_l}[\tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})] = \sum_{\beta_l+\gamma_l=2\alpha_l}(2\alpha_l)!\frac{D^{\beta_l}\tilde{u}_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})}{\beta_l!}\frac{D^{\gamma_l}\tilde{u}_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})}{\gamma_l!},
$$

and thus by (5.29) and the fact that $\sum_{\beta_l+\gamma_l=2\alpha_l}\frac{(2\alpha_l)!}{\beta_l!\gamma_l!} = 2^{2|\alpha_l|-1}$, we have

$$
\begin{aligned}
\left|D^{2\alpha_l}[\tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})]\right| &\le 2^{2|\alpha_l|-1}(C\Delta^{1-\epsilon})^{|\alpha_l|}\mathbb{E}_Q[U^2_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})]\prod_{k=2}^{l}(k-1)^{(\varepsilon-1)\alpha_l^k} \\
&\quad\times\max_{\beta_l+\gamma_l=2\alpha_l}\left(\left(\mathbb{E}_Q\left[\left|\nu_1(\hat{X}_{\Delta,x}(\cdot))\right|^{2|\beta_l|}_{\frac{1-\varepsilon}{2},2,[0,\Delta]}\right]\right)^{1/2}\right. \\
&\quad\left.\times\left(\mathbb{E}_Q\left[\left|\nu_1(\hat{X}_{\Delta,x}(\cdot))\right|^{2|\gamma_l|}_{\frac{1-\varepsilon}{2},2,[0,\Delta]}\right]\right)^{1/2}\right).
\end{aligned}
$$

Similar to (5.22), we have $\mathbb{E}_Q\left[|\nu_1(\hat{X}_{\Delta,x}(\cdot))|^{2|\beta_l|}_{\frac{1-\varepsilon}{2},2,[0,\Delta]}\right] \le C(\Delta^{|\beta_l|(2+\varepsilon)} + \Delta^{|\beta_l|(1+\varepsilon)})$ and

$$
(5.30)\quad \left|D^{2\alpha_l}[\tilde{u}^2_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})]\right| \le C(\Delta^{3|\alpha_l|}+\Delta^{2|\alpha_l|})\prod_{k=2}^{l}(k-1)^{(\varepsilon-1)\alpha_l^k}\mathbb{E}_Q[U^2_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})].
$$

Then by (5.28) and (5.30), we obtain

$$
\begin{aligned}
&\left|S(\mathsf{L},l)\otimes_{n=l+1}^{\mathsf{n}} I_1^{(n)}\varphi\right| \\
&\quad\le C(\Delta^{3\mathsf{L}}+\Delta^{2\mathsf{L}})(1+(3c/2)^{L\wedge l})\beta^{-(\mathsf{L}\wedge l)/2} \\
&\qquad\times\mathbb{E}[\mathbb{E}_Q[U^2_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})]]\sum_{i_1+\cdots+i_l=\mathsf{L}+l-1}\prod_{k=2}^{l}(k-1)^{(\varepsilon-1)\alpha_l^k} \\
(5.31)\qquad&\quad\le C(\Delta^{3\mathsf{L}}+\Delta^{2\mathsf{L}})(1+(3c/2)^{L\wedge l})\beta^{-(\mathsf{L}\wedge l)/2}\epsilon^{1-\mathsf{L}}(l-1)^{\mathsf{L}\varepsilon-1}
\end{aligned}
$$

with the constant $C>0$ which does not depend on n, ε, L, c, β, and l. In the last line we used the fact that $\mathbb{E}[\mathbb{E}_Q[U^2_{\Delta,\mathsf{n}}(\Delta,x,\mathbf{y})]]$ is bounded and that

$$\sum_{i_1+\cdots+i_l=\mathsf{L}+l-1}\prod_{k=2}^{l}(k-1)^{(\varepsilon-1)\alpha_l^k} = (l-1)^{\varepsilon-1}\sum_{i_1+\cdots+i_l=\mathsf{L}+l-1}\prod_{k=2}^{l}(k-1)^{(\varepsilon-1)(i_k-1)}$$
$$\le (l-1)^{\varepsilon-1}\left(\sum_{k=2}^{l}(k-1)^{\varepsilon-1}\right)^{\mathsf{L}-1} \le (l-1)^{\varepsilon-1}(\varepsilon^{-1}(l-1)^{\varepsilon})^{\mathsf{L}-1} = \varepsilon^{1-\mathsf{L}}(l-1)^{\mathsf{L}\varepsilon-1}.$$

Then by (5.26) and (5.31), we have

$$\begin{aligned}|I_{\mathsf{n}}\varphi - A(\mathsf{L},\mathsf{n})\varphi| &\le C(\Delta^{3\mathsf{L}}+\Delta^{2\mathsf{L}})(1+(3c/2)^{L\wedge\mathsf{n}})\beta^{-(\mathsf{L}\wedge\mathsf{n})/2}\epsilon^{1-\mathsf{L}}\sum_{l=2}^{\mathsf{n}}(l-1)^{L\varepsilon-1}\\ &\quad + \left|(I_1^{(1)}-Q_{\mathsf{L}}^{(1)})\otimes_{k=2}^{\mathsf{n}} I_1^{(k)}\varphi\right|\\ &\le C(\Delta^{3\mathsf{L}}+\Delta^{2\mathsf{L}})(1+(3c/2)^{\mathsf{L}\wedge\mathsf{n}})\beta^{-(\mathsf{L}\wedge\mathsf{n})/2}\varepsilon^{-\mathsf{L}}\mathsf{L}^{-1}\mathsf{n}^{\mathsf{L}\varepsilon},\end{aligned}$$

where the term in the second line is estimated by the classical error estimate for the Gauss–Hermite quadrature Q (see, e.g., [24]) and the estimation of derivatives (5.30).

The global error is estimated from the recursion nature of Algorithm 2.2 as in the proof in [21, Theorem 2.4]. ∎

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