A MULTILEVEL MONTE CARLO ENSEMBLE SCHEME FOR SOLVING RANDOM PARABOLIC PDES

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Abstract. A first-order, Monte Carlo ensemble method has been recently introduced for solving parabolic equations with random coefficients in [26], which is a natural synthesis of the ensemble-based, Monte Carlo sampling algorithm and the ensemble-based, first-order time stepping scheme. With the introduction of an ensemble average of the diffusion function, this algorithm leads to a single discrete system with multiple right-hand sides for a group of realizations, which could be solved more efficiently than a sequence of linear systems. In this paper, we pursue in the same direction and develop a new multilevel Monte Carlo ensemble method for solving random parabolic partial differential equations. Comparing with the approach in [26], this method possesses a second-order accuracy in time and further reduces the computational cost by using the multilevel Monte Carlo sampling method. Rigorous numerical analysis shows the method achieves the optimal rate of convergence. Several numerical experiments are presented to illustrate the theoretical results.

Key words. ensemble-based time stepping, multilevel Monte Carlo, random parabolic PDEs

1. Introduction.

In this paper, we consider numerical solutions to the following unsteady heat conduction equation in a random, spatially varying medium: to find a random function, $u : \Omega \times \overline{D} \times [0, T] \to \mathbb{R}$ satisfying almost surely (a.s.)

$$
(1) \qquad \begin{cases} u_t(\omega, \mathbf{x}, t) - \nabla \cdot [(a(\omega, \mathbf{x})\nabla u(\omega, \mathbf{x}, t)] = f(\omega, \mathbf{x}, t), & \text{in } \Omega \times D \times [0, T] \\ u(\omega, \mathbf{x}, t) = g(\omega, \mathbf{x}, t), & \text{on } \Omega \times \partial D \times [0, T] \\ u(\omega, \mathbf{x}, 0) = u^0(\omega, \mathbf{x}), & \text{in } \Omega \times D \end{cases},
$$

where D is a bounded Lipschitz domain in $\mathbb{R}^d$ ($d = 1, 2,$ or 3) and $(\Omega, \mathcal{F}, P)$ is a probability space with the sample space Ω, σ-algebra $\mathcal{F}$, and probability measure P; diffusion coefficient $a : \Omega \times D \to \mathbb{R}$ and body force $f : \Omega \times D \times [0, T] \to \mathbb{R}$ are random fields with continuous and bounded covariance functions.

Many numerical methods, either intrusive or non-intrusive, have been developed for random partial differential equations (PDEs), see, e.g., in the review papers [16, 40] and the references therein. For the random steady or unsteady heat equation, non-intrusive numerical methods such as Monte Carlo methods are known for easy implementation but requiring a very large number of PDE solutions to achieve small errors; while intrusive methods such as the stochastic Galerkin or collocation approaches can achieve faster convergence but would require the solution of discrete systems that couple all spatial and probabilistic degrees of freedom [2, 3, 41]. To improve the computational efficiency of the non-intrusive approaches, other sampling methods such as quasi-Monte Carlo, multilevel Monte Carlo (MLMC), Latin hypercube sampling and Centroidal Voronoi tessellations can be used [29, 19, 8, 35]. In particular, the MLMC method is designed to greatly reduce the computational cost by performing most simulations at a low accuracy, while running relatively few simulations at a

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high accuracy. It was first introduced by Heinrich [18] for the computation of high-dimensional, parameter-dependent integrals and was analyzed extensively by Giles [11, 10] in the context of stochastic differential equations in mathematical finance. In [7], Cliffe et al. applied the MLMC method to the elliptic PDEs with random coefficients and demonstrated its numerical superiority. Under the assumptions of uniform coercivity and boundedness of the random parameter, numerical error of the MLMC approximation has been analyzed in [4]. The result was extended in [5] for random elliptic problems with weaker assumptions on the random parameter and a limited spatial regularity.

Overall, the above mentioned sampling methods are ensemble-based. To quantify probabilistic uncertainties in a system governed by random PDEs, an ensemble of independent realizations of the random parameters needs to be considered. In practice, this process would involve solving a group of deterministic PDEs corresponding to all the realizations. A straightforward solution strategy is to find numerical approximate solutions of the deterministic PDEs from a sequence of discrete linear systems. Obviously, this approach ignores any possible relationships among the group members, thus cannot improve the overall computational efficiency. To speed up the group of simulations, current active research mainly starts from the perspective of numerical linear algebra, and develops iterative algorithms that can take advantage of the relationship in the sequence of discrete systems. For instance, subspace recycling techniques such as GCRO with deflated restarting have been introduced in [33] for accelerating the solutions of slowly-changing linear systems, which is further developed in [1] for climate modeling and uncertainty quantification applications. For sequences sharing a common coefficient matrix, block iterative algorithms [17, 27, 31, 32, 36] have been developed to solve the system with many right-hand sides. The algorithms have been used to accelerate convergence even when there is only one right-hand side in [6, 32]. The block version of GCRO with deflated restarting was introduced in [34], and its high-performance implementation is available in the Belos package of the Trilinos project developed at US Sandia National Laboratories.

Recently, the Monte Carlo ensemble method was introduced by the authors of this paper for solving the random heat equations in [26]. This method is motivated by the ensemble-based time stepping algorithm, which was proposed for solving Navier-Stokes incompressible flow ensembles in [23, 20, 22, 24, 37, 21] and for simulating ensembles of parameterized Navier-Stokes flow problems in [14, 15]. It has been extended to MHD flows in [28] and to low-dimensional surrogate models in [12, 13]. The main idea is to manipulate the numerical scheme so that all the simulations in the ensemble could share a common coefficient matrix. As a consequence, simulating the ensemble only requires to solve a single linear system with multiple right-hand sides, which could be easily handled by a block iterative solver and, thus, improves the overall computational efficiency. Thus, the Monte Carlo ensemble method was proposed in [26] for synthesizing a first-order, ensemble-based time-stepping and the ensemble-based, Monte Carlo sampling method in a natural way, which speeds up the numerical approximation of the random parabolic PDE solutions and other possible quantities of interest. However, it is known that the Monte Carlo method, although easy for implementations, is a computationally expensive random sampling approach. Therefore, we develop a new method for solving the same random heat equations with a better accuracy and efficiency in this paper: the new method is second-order accurate in time, which improves the temporal accuracy of our previous work; it employs the idea of multilevel Monte Carlo methods, which improves the sampling efficiency comparing with the Monte Carlo. We further perform theoretical analysis on the method and present numerical tests that illustrate our theoretical findings. Upon the completion of this paper, we found the second-order ensemble-based time-stepping scheme had been used in [9] for solving heat equation with uncertain conductivity, however, without discussing the sampling error in their analysis.

The rest of this paper is organized as follows. In Section 2, we present some notation and mathematical preliminaries. In Section 3, we introduce the multilevel Monte Carlo ensemble scheme in the context of finite element (FE) methods. In Section 4, we analyze the proposed algorithm, prove its stability and convergence, and discuss its computational complexity. Numerical experiments are presented in Section 5, which illustrate the effectiveness of the proposed scheme on random parabolic problems. A few concluding remarks are given in Section 6.

2. Notation and preliminaries. Denote the $L^2(D)$ norm and inner product by $\|\cdot\|$ and $(\cdot,\cdot)$, respectively. Let $W^{s,q}(D)$ be the Sobolev space of functions having generalized derivatives up to the order s in the space $L^q(D)$, where s is a nonnegative integer and $1 \le q \le +\infty$. The equipped Sobolev norm of $v \in W^{s,q}(D)$ is denoted by $\|v\|_{W^{s,q}(D)}$. When $q = 2$, we use the notation $H^s(D)$ instead of $W^{s,2}(D)$. As usual, the function space $H_0^1(D)$ is the subspace of $H^1(D)$ consisting of functions that vanish on the boundary of D in the sense of trace, equipped with the norm $\|v\|_{H_0^1(D)} = \left(\int_D |\nabla v|^2 \, d\mathbf{x}\right)^{1/2}$. When $s = 0$, we shall keep the notation with $L^q(D)$ instead of $W^{0,q}(D)$. The space $H^{-s}(D)$ is the dual space of bounded linear functions on $H_0^s(D)$. A norm for $H^{-1}(D)$ is defined by $\|f\|_{-1} = \sup\limits_{0\neq v\in H_0^1(D)} \frac{(f,v)}{\|\nabla v\|}$.

Let $(\Omega, \mathcal{F}, P)$ be a complete probability space. If Y is a random variable in the space that belongs to $L_P^1(\Omega)$, its expected value is defined by

$$\mathbb{E}[Y] = \int_\Omega Y(\omega) dP(\omega).$$

With the multi-index notation, $\alpha = (\alpha_1, \dots, \alpha_d)$ is a d-tuple of nonnegative integers with the length $|\alpha| = \sum_{i=1}^d \alpha_i$. The stochastic Sobolev space $\widetilde{W}^{s,q}(D) = L_P^q(\Omega, W^{s,q}(D))$ containing stochastic functions, $v : \Omega \times D \to R$, that are measurable with respect to the product σ-algebra $\mathcal{F} \bigotimes B(D)$ and equipped with the averaged norms $\|v\|_{\widetilde{W}^{s,q}(D)} = \left(\mathbb{E}[\|v\|^q_{W^{s,q}(D)}]\right)^{1/q} = \left(\mathbb{E}[\sum_{|\alpha|\le s} \int_D |\partial^\alpha v|^q d\mathbf{x}]\right)^{1/q}, 1 \le q < +\infty$. Observe that if $v \in \widetilde{W}^{s,q}(D)$, then $v(\omega, \cdot) \in W^{s,q}(D)$ a.s. and $\partial^\alpha v(\cdot, x) \in L_P^q(\Omega)$ a.e. on D for $|\alpha| < s$. In particular, we consider the Hilbert space $\widetilde{L}^2(H^s(D); 0, T)$ of stochastic functions $v : \Omega \times D \times [0, T] \to R$, in which any element v belongs to $\widetilde{H}^s(D)$ for each $0 \le t \le T$ with the property that $\|v\|_{\widetilde{W}^{s,q}(D)}$ is square integrable on $[0, T]$; and $\widetilde{H}^s(L^2(D); 0, T)$ in which any element v belongs to $\widetilde{L}^2(D)$ for each $0 \le t \le T$ with the property that $\|v\|_{\widetilde{L}^2(D)}$ belongs to $H^s(0, T)$.

3. Multilevel Monte Carlo ensemble method. Given statistical information on the inputs of a random/stochastic PDE, uncertainty quantification fulfills the task of determining statistical information about outputs of interest that depend on the PDE solutions. When stochastic sampling methods such as the Monte Carlo are used to solve (1), one has to find approximate solutions associated to an ensemble of independent realizations, that is, deterministic PDEs at randomly selected sample values. Usually, numerical simulations are implemented separately, thus the total computational cost is simply multiplied as the sampling set grows. To improve the efficiency, we propose an ensemble-based multilevel Monte Carlo method in this paper, which is an extension of the Monte Carlo ensemble method we introduced in [26]. The new approach outperforms the previous one in both accuracy and efficiency, which is due to the combination of a second-order, ensemble-based time stepping scheme and the multilevel Monte Carlo method.

Next, we present the algorithm in the context of numerical solutions to the random PDE (1). For the spatial discretization, we use conforming finite elements, although other numerical methods could be applied as well. To fit in the hierarchic nature of multilevel Monte Carlo methods, we consider a sequence of quasi-uniform meshes comprising a set of shape-regular triangles (or tetrahedra), $\{\mathcal{T}_l\}_{l=0}^L$, for a polygonal (or polyhedral) domain D. Denote the mesh size of $\mathcal{T}_l$ by

$$h_l = \max_{K\in\mathcal{T}_l} \operatorname{diam} K.$$

Assume the sequence of meshes is generated by uniform refinements satisfying

$$h_l = 2^{-l} h_0. \tag{2}$$

Define the function space $H_g^1(D) = \{v \in H^1(D) : v|_{\partial D} = g\}$ and the FE space

$$V_l^g := \{v \in H_g^1(D) \cap H^{m+1}(D) : v|_K \text{ is a polynomial of degree } m, \forall K \in \mathcal{T}_l\}$$

for a non-negative integer m. The sequence of finite element spaces satisfies

$$V_0^g \subset V_1^g \subset \cdots \subset V_l^g \subset \cdots \subset V_L^g.$$

Denoted by $u_l(\omega, \mathbf{x}, t_n)$ the finite element solution in V_l^g at the time instance t_n. The MLMC FE solution at the L-th level mesh can be written as

$$u_L(\omega, \mathbf{x}, t_n) = \sum_{l=1}^{L} \big(u_l(\omega, \mathbf{x}, t_n) - u_{l-1}(\omega, \mathbf{x}, t_n)\big) + u_0(\omega, \mathbf{x}, t_n).$$

Based on linearity of the expectation operator $\mathbb{E}[\cdot]$, we have

$$\begin{aligned}\mathbb{E}\big[u_L(\omega, \mathbf{x}, t_n)\big] &= \mathbb{E}\Big[\sum_{l=1}^{L} \big(u_l(\omega, \mathbf{x}, t_n) - u_{l-1}(\omega, \mathbf{x}, t_n)\big) + u_0(\omega, \mathbf{x}, t_n)\Big] \\ &= \sum_{l=1}^{L} \mathbb{E}\big[u_l(\omega, \mathbf{x}, t_n) - u_{l-1}(\omega, \mathbf{x}, t_n)\big] + \mathbb{E}\big[u_0(\omega, \mathbf{x}, t_n)\big].\end{aligned}$$

Numerically, the expected value of the FE solution on the l-th level, $\mathbb{E}[u_l(\omega, \mathbf{x}, t_n)]$ is approximated by the sampling average $\Psi_{J_l}^n = \Psi_{J_l}[u_l(\omega, \mathbf{x}, t_n)] = \frac{1}{J_l}\sum_{j=1}^{J_l} u_l(\omega_j, \mathbf{x}, t_n)$, where J_l is the sample size. Correspondingly, $\mathbb{E}[u_L(\omega, \mathbf{x}, t_n)]$ is approximated by an unbiased estimator:

$$\Psi[u_L(\omega, \mathbf{x}, t_n)] := \sum_{l=1}^{L} \big(\Psi_{J_l}[u_l(\omega, \mathbf{x}, t_n) - u_{l-1}(\omega, \mathbf{x}, t_n)]\big) + \Psi_{J_0}[u_0(\omega, \mathbf{x}, t_n)]. \tag{3}$$

It is seen that, at each mesh level, a group of simulations needs to be implemented. Thus, it is natural to extend ensemble-based time stepping to such settings for reducing the computational cost. Next, we introduce the multilevel Monte Carlo ensemble (MLMCE) method to achieve this goal.

For simplicity of presentation, we assume that, at the l-th level, a uniform time partition with the time step Δt_l is used for the simulations and further set $N_l = T/\Delta t_l$; J_l independent, identically distributed (i.i.d.) samples are selected, and the associated random functions are denoted by $a_j \equiv a(\omega_j, \cdot)$, $f_j \equiv f(\omega_j, \cdot, \cdot)$, $g_j \equiv g(\omega_j, \cdot, \cdot)$, and $u_j^0 \equiv u^0(\omega_j, \cdot)$ for $j = 1, \ldots, J_l$, and define the ensemble mean of the diffusion coefficient functions by

$$\overline{a}_l := \frac{1}{J_l} \sum_{j=1}^{J_l} a(\omega_j, \mathbf{x}).$$

Here, we note that the corresponding exact solutions $\{u(\omega_j, \mathbf{x}, t)\}_{j=1}^{J_l}$ are i.i.d. Let $u_{j,l}^n = u_l(\omega_j, \mathbf{x}, t_n)$, the finite element approximation of $u(\omega_j, \mathbf{x}, t_n)$ at the l-th level.

The *multilevel Monte Carlo ensemble method (MLMCE)* applied to (1) solves the following group of simulations at the l-th level: for $j = 1, \ldots, J_l$, given $u_{j,l}^0$ and $u_{j,l}^1$, to find $u_{j,l}^{n+1} \in V_l^g$ such that,

$$\begin{aligned} (4) \qquad & \left(\frac{3u_{j,l}^{n+1} - 4u_{j,l}^n + u_{j,l}^{n-1}}{2\Delta t_l}, v_l \right) + (\overline{a}_l \nabla u_{j,l}^{n+1}, \nabla v_l) \\ & = -\big((a_j - \overline{a}_l)\nabla(2u_{j,l}^n - u_{j,l}^{n-1}), \nabla v_l\big) + (f_j^{n+1}, v_l), \quad \forall\, v_l \in V_l^0, \end{aligned}$$

for $n = 1, \ldots, N_l - 1$. Once the numerical solutions at all the L levels are found, the MLMCE approximates the random PDE solution at the time instance t_n, $\mathbb{E}[u(t_n)]$, by (3). Meanwhile, given a quantity of interest $Q(u)$, one can analyze the outputs from the ensemble simulations, $Q(u_h(\omega_1, \cdot, \cdot)), \ldots, Q(u_h(\omega_J, \cdot, \cdot))$, to extract the underlying stochastic information of the system.

The MLMCE naturally combines the ensemble-based sampling method and the ensemble-based time stepping algorithm, and inherits advantages from both sides. As the MLMC, the method can reduce the computational cost by balancing the time step size, mesh size, and the number of samples at each level. Meanwhile, the ensemble-based time stepping algorithm leads to a discrete linear system (4) whose coefficient matrix is independent of j. Indeed, denote the mass matrix by $\mathbf{M}_l$ that is associated with (v_l, v_l) and the stiffness matrix $\mathbf{S}_l$ that is related to $(\overline{a}_l \nabla v_l, \nabla v_l)$, the coefficient matrix of (4) is $\frac{3}{2\Delta t}\mathbf{M}_l + \mathbf{S}_l$. Hence, for evaluating J_l realizations, one only needs to solve one linear system with J_l right-hand sides, which leads to great computational savings comparing with a sequence of individual simulations: when the number of degrees of freedom is small, one only need to perform the LU factorization once instead of J_l times; when the number of degrees of freedom is large, one can use the block iterative algorithms to accelerate solutions. Next, we will analyze the stability and asymptotic error estimate of the MLMCE method.

4. Stability and error estimate. To simplify the presentation, we only consider equation (1) with the homogeneous boundary condition (that is, $g = 0$ and $u_{j,l}^{n+1} \in V_l^0$ in the FE weak form (4)), while the nonhomogeneous cases can be similarly analyzed by incorporating the method of shifting. Meanwhile, we will include numerical test cases with nonhomogeneous boundary conditions in Section 5. As the MLMCE approximation is based on the MC solutions at various levels, we first analyze the ensemble-based single-level Monte Carlo in Subsection 4.1 and derive the error estimate for MLMCE in Subsection 4.2.

Assume the exact solution of (1) is smooth enough, in particular,

$$u_j \in \widetilde{L}^2(H_0^1(D) \cap H^{m+1}(D); 0, T) \cap \widetilde{H}^1(H^{m+1}(D); 0, T) \cap \widetilde{H}^2(L^2(D); 0, T)$$

and suppose

$$f_j \in \widetilde{L}^2\left(H^{-1}(D); 0, T\right).$$

Here we use the notation introduced in Section 2. We emphasize the assumed regularity only requires the random fields to be square integrable. Assume the following two conditions hold:

(i) There exists a positive constant θ such that

$$P\{\omega \in \Omega; \min_{\mathbf{x}\in\overline{D}} a(\omega, \mathbf{x}) > \theta\} = 1.$$

(ii) There exists a positive constant θ_+, for $l = 0, \dots, L$, such that

$$P\{\omega_j \in \Omega; |a(\omega, \mathbf{x}) - \overline{a}_l|_\infty \le \theta_+\} = 1.$$

Here, condition (i) guarantees the uniform coercivity a.s. and condition (ii) gives an upper bound of the distance from coefficient $a(\omega, \mathbf{x})$ to the ensemble average $\overline{a}_l$ a.s.

4.1. Single-level Monte Carlo ensemble finite element method. When $\mathbb{E}[u(t_n)]$ is numerically approximated by $\Psi^n_{J_l}$, the associated approximation error can be separated into two parts:

$$\mathbb{E}[u(t_n)] - \Psi^n_{J_l} = \left(\mathbb{E}[u_j(t_n)] - \mathbb{E}[u^n_{j,l}]\right) + \left(\mathbb{E}[u^n_{j,l}] - \Psi^n_{J_l}\right) := \mathcal{E}^n_l + \mathcal{E}^n_S,$$

where we use the fact that $\mathbb{E}[u(t_n)] = \mathbb{E}[u_j(t_n)]$. The finite element discretization error, $\mathcal{E}^n_l = \mathbb{E}[u_j(t_n) - u^n_{j,l}]$, is controlled by the size of spatial triangulations $\mathcal{T}_l$ and time step; while the statistical sampling error, $\mathcal{E}^n_S = \mathbb{E}[u^n_{j,l}] - \Psi^n_{J_l}$, is dominated by the number of realizations and variance. Next, we will first discuss the stability of the ensemble scheme (4) at the l-th level (Theorem 1), derive the bounds for $\mathcal{E}^n_S$ (Theorem 3) and $\mathcal{E}^n_l$ (Theorem 4), and then obtain the asymptotic error estimation (Theorem 5).

THEOREM 1. *Under conditions* (i) *and* (ii)*, the scheme (4) is stable provided that*

$$\theta > 3\theta_+. \tag{5}$$

Furthermore, the numerical solution to (4) satisfies

$$\begin{aligned}
&\frac{1}{4}\mathbb{E}\big[\|u^{N_l}_{j,l}\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2u^{N_l}_{j,l} - u^{N_l-1}_{j,l}\|^2\big] + \Big(\frac{\theta}{3} - \theta_+\Big)\Delta t_l \sum_{n=1}^{N_l} \mathbb{E}\big[\|\nabla u^n_{j,l}\|^2\big] \\
&\le \frac{\Delta t_l}{2(\theta - 3\theta_+)} \sum_{n=1}^{N_l-1} \mathbb{E}\big[\|f^{n+1}_j\|^2_{-1}\big] + \frac{1}{4}\mathbb{E}\big[\|u^1_{j,l}\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2u^1_{j,l} - u^0_{j,l}\|^2\big] \\
&+ \frac{\theta}{2}\Delta t_l \mathbb{E}\big[\|\nabla u^1_{j,l}\|^2\big] + \frac{\theta}{6}\Delta t_l \mathbb{E}\big[\|\nabla u^0_{j,l}\|^2\big].
\end{aligned} \tag{6}$$

Proof. Choosing $v_h = u^{n+1}_{j,l}$ in (4), we obtain

$$\begin{aligned}
&\left(\frac{3u^{n+1}_{j,l} - 4u^n_{j,l} + u^{n-1}_{j,l}}{2\Delta t_l}, u^{n+1}_{j,l}\right) + \left(\overline{a}_l \nabla u^{n+1}_{j,l}, \nabla u^{n+1}_{j,l}\right) \\
&\quad = -\left((a_j - \overline{a}_l)\nabla(2u^n_{j,l} - u^{n-1}_{j,l}), \nabla u^{n+1}_{j,l}\right) + \left(f^{n+1}_j, u^{n+1}_{j,l}\right).
\end{aligned} \tag{7}$$

Multiplying both sides by Δt_l, integrating over the probability space and considering the coercivity, we get

$$
\begin{aligned}
&\frac{1}{4}\mathbb{E}\big[\|u_{j,l}^{n+1}\|^2 + \|2u_{j,l}^{n+1} - u_{j,l}^{n}\|^2\big] - \frac{1}{4}\mathbb{E}\big[\|u_{j,l}^{n}\|^2 + \|2u_{j,l}^{n} - u_{j,l}^{n-1}\|^2\big] \\
&+ \frac{1}{4}\mathbb{E}\big[\|u_{j,l}^{n+1} - 2u_{j,l}^{n} + u_{j,l}^{n-1}\|^2\big] + \Delta t_l \theta\, \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2\big] \\
&\le \Delta t_l \mathbb{E}\big[\big|\big(f_j^{n+1}, u_{j,l}^{n+1}\big)\big|\big] + \Delta t_l \theta_+ \mathbb{E}\big[\big|\big(\nabla(2u_{j,l}^{n} - u_{j,l}^{n-1}), \nabla u_{j,l}^{n+1}\big)\big|\big].
\end{aligned} \tag{8}
$$

Apply Young's inequality to the terms on the right-hand side (RHS), we have, for any $\beta_i > 0, i = 1, 2, 3$,

$$
\mathbb{E}\big[\big|(f_j^{n+1}, u_{j,l}^{n+1})\big|\big] \le \frac{\beta_1}{4}\mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2\big] + \frac{1}{\beta_1}\mathbb{E}\big[\|f_j^{n+1}\|_{-1}^2\big], \tag{9}
$$

and

$$
\begin{aligned}
&\mathbb{E}\Big[\big|\big(\nabla(2u_{j,l}^{n} - u_{j,l}^{n-1}), \nabla u_{j,l}^{n+1}\big)\big|\Big] = \mathbb{E}\Big[\big|(2\nabla u_{j,l}^{n}, \nabla u_{j,l}^{n+1}) - (\nabla u_{j,l}^{n-1}, \nabla u_{j,l}^{n+1})\big|\Big] \\
&\le \frac{\beta_2 + \beta_3}{2}\mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2\big] + \frac{2}{\beta_2}\mathbb{E}\big[\|\nabla u_{j,l}^{n}\|^2\big] + \frac{1}{2\beta_3}\mathbb{E}\big[\|\nabla u_{j,l}^{n-1}\|^2\big].
\end{aligned} \tag{10}
$$

The term $\Delta t_l \theta \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2\big]$ on the left-hand side (LHS) can be split into several parts, for any $C_1 \in (0, 1)$:

$$
\begin{aligned}
\Delta t_l \theta \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2\big] &= C_1 \Delta t_l \theta \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2\big] + (1 - C_1)\Delta t_l \theta \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2 - \|\nabla u_{j,l}^{n}\|^2\big] \\
&\quad + (1 - C_1)\Delta t_l \theta \mathbb{E}\big[\|\nabla u_{j,l}^{n}\|^2\big].
\end{aligned} \tag{11}
$$

Substituting (9)-(11) into (8), we get

$$
\begin{aligned}
&\frac{1}{4}\big(\mathbb{E}\big[\|u_{j,l}^{n+1}\|^2\big] + \mathbb{E}\big[\|2u_{j,l}^{n+1} - u_{j,l}^{n}\|^2\big]\big) - \frac{1}{4}\big(\mathbb{E}\big[\|u_{j,l}^{n}\|^2\big] + \mathbb{E}\big[\|2u_{j,l}^{n} - u_{j,l}^{n-1}\|^2\big]\big) \\
&+ \frac{1}{4}\mathbb{E}\big[\|u_{j,l}^{n+1} - 2u_{j,l}^{n} + u_{j,l}^{n-1}\|^2\big] + \Big(C_1\theta - \frac{\beta_1}{4} - \frac{\beta_2 + \beta_3}{2}\theta_+\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2\big] \\
&+ (1 - C_1)\Delta t_l \theta \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2 - \|\nabla u_{j,l}^{n}\|^2\big] + \Big(\frac{2}{3}(1 - C_1)\theta - \frac{2\theta_+}{\beta_2}\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n}\|^2\big] \\
&+ \Big(\frac{1}{3}(1 - C_1)\theta\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n}\|^2 - \|\nabla u_{j,l}^{n-1}\|^2\big] \\
&+ \Big(\frac{1}{3}(1 - C_1)\theta - \frac{\theta_+}{2\beta_3}\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n-1}\|^2\big] \le \frac{\Delta t_l}{\beta_1}\mathbb{E}\big[\|f_j^{n+1}\|_{-1}^2\big].
\end{aligned} \tag{12}
$$

Selecting $\beta_1 = 4\delta\theta_+$, $\beta_2 = 2$, and $\beta_3 = 1$ for some positive δ, (12) becomes

$$
\begin{aligned}
&\frac{1}{4}\mathbb{E}\big[\|u_{j,l}^{n+1}\|^2 + \|2u_{j,l}^{n+1} - u_{j,l}^{n}\|^2\big] - \frac{1}{4}\mathbb{E}\big[\|u_{j,l}^{n}\|^2 + \|2u_{j,l}^{n} - u_{j,l}^{n-1}\|^2\big] \\
&+ \frac{1}{4}\mathbb{E}\big[\|u_{j,l}^{n+1} - 2u_{j,l}^{n} + u_{j,l}^{n-1}\|^2\big] + \Big(C_1\theta - \frac{2\delta + 3}{2}\theta_+\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2\big] \\
&+ (1 - C_1)\Delta t_l \theta \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2 - \|\nabla u_{j,l}^{n}\|^2\big] + \Big(\frac{2}{3}(1 - C_1)\theta - \theta_+\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n}\|^2\big] \\
&+ \Big(\frac{1}{3}(1 - C_1)\theta\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n}\|^2 - \|\nabla u_{j,l}^{n-1}\|^2\big] \\
&+ \Big(\frac{1}{3}(1 - C_1)\theta - \frac{\theta_+}{2}\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n-1}\|^2\big] \le \frac{\Delta t_l}{4\delta\theta_+}\mathbb{E}\big[\|f_j^{n+1}\|_{-1}^2\big].
\end{aligned} \tag{13}
$$

Stability follows if the following conditions hold:

$$C_1\theta - \frac{2\delta+3}{2}\theta_+ \geq 0, \tag{14}$$

$$\frac{1}{3}(1-C_1)\theta - \frac{\theta_+}{2} \geq 0. \tag{15}$$

By taking $C_1 = \frac{1}{2}$ and $\delta = \frac{\theta - 3\theta_+}{2\theta_+}$, under the assumption (5), we have

$$C_1\theta - \frac{2\delta+3}{2}\theta_+ = \frac{\theta}{2} - \frac{\theta}{2} = 0 \quad \text{and} \quad \frac{\theta}{3} - \theta_+ > 0.$$

Then, by dropping a positive term, (13) becomes

$$\begin{aligned}
&\frac{1}{4}\mathbb{E}\big[\|u_{j,l}^{n+1}\|^2 + \|2u_{j,l}^{n+1} - u_{j,l}^n\|^2\big] - \frac{1}{4}\mathbb{E}\big[\|u_{j,l}^n\|^2 + \|2u_{j,l}^n - u_{j,l}^{n-1}\|^2\big] \\
&+ \frac{\theta}{2}\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n+1}\|^2 - \|\nabla u_{j,l}^n\|^2\big] + \Big(\frac{\theta}{3} - \theta_+\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^n\|^2\big] \\
&+ \frac{\theta}{6}\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^n\|^2 - \|\nabla u_{j,l}^{n-1}\|^2\big] + \Big(\frac{\theta}{6} - \frac{\theta_+}{2}\Big)\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^{n-1}\|^2\big] \\
&\leq \frac{\Delta t_l}{2(\theta - 3\theta_+)}\mathbb{E}\big[\|f_j^{n+1}\|_{-1}^2\big].
\end{aligned} \tag{16}$$

Summing (16) from $n = 1$ to $n = N_l - 1$ and dropping two positive terms gives

$$\begin{aligned}
&\frac{1}{4}\mathbb{E}\big[\|u_{j,l}^{N_l}\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2u_{j,l}^{N_l} - u_{j,l}^{N_l-1}\|^2\big] + \Big(\frac{\theta}{3} - \theta_+\Big)\Delta t_l \sum_{n=1}^{N_l} \mathbb{E}\big[\|\nabla u_{j,l}^n\|^2\big] \\
&\leq \frac{\Delta t_l}{2(\theta - 3\theta_+)} \sum_{n=1}^{N_l-1} \mathbb{E}\big[\|f_j^{n+1}\|_{-1}^2\big] + \frac{1}{4}\mathbb{E}\big[\|u_{j,l}^1\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2u_{j,l}^1 - u_{j,l}^0\|^2\big] \\
&+ \frac{\theta}{2}\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^1\|^2\big] + \frac{\theta}{6}\Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^0\|^2\big],
\end{aligned} \tag{17}$$

which completes the proof. ∎

Remark 2. *The ensemble-based time stepping scheme (4) is stable if condition (5) is satisfied. Moreover, it becomes to be unconditionally stable when the size of ensemble equals one since θ_+ would shrink to zero. Thus, given a group of problems, one can use condition (5) as a guideline to divide problems into subgroups so that condition (5) holds in each of them. The smallest subgroup could contain only one member for that no stability condition is required.*

Next, by using the standard error estimate for the Monte Carlo method (e.g., [25]), we can bound the statistical error $\mathcal{E}_S^n$ as follows.

Theorem 3. *Let $\mathcal{E}_S^n = \mathbb{E}[u_{j,l}^n] - \Psi_{J_l}^n$, where $u_{j,l}^n$ is the result of scheme (4) and $\Psi_{J_l}^n = \frac{1}{J_l}\sum_{j=1}^{J_l} u_{j,l}^n$. Suppose conditions* (i) *and* (ii)*, and the stability condition (5) hold, there is a generic positive constant C independent of J_l, h_l and Δt_l such that*

$$\begin{aligned}
&\frac{1}{4}\mathbb{E}\big[\|\mathcal{E}_S^{N_l}\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2\mathcal{E}_S^{N_l} - \mathcal{E}_S^{N_l-1}\|^2\big] + \left(\frac{\theta}{3} - \theta_+\right)\Delta t_l \sum_{n=1}^{N_l} \mathbb{E}\big[\|\nabla \mathcal{E}_S^n\|^2\big] \\
&\leq \frac{C}{J_l}\Big(\Delta t_l \sum_{n=1}^{N_l} \mathbb{E}\big[\|f_j^n\|_{-1}^2\big] + \Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^1\|^2\big] + \mathbb{E}\big[\|\nabla u_{j,l}^0\|^2\big] \\
&+ \mathbb{E}\big[\|u_{j,l}^1\|^2\big] + \mathbb{E}\big[\|2u_{j,l}^1 - u_{j,l}^0\|^2\big]\Big).
\end{aligned} \tag{18}$$

Proof. First, we estimate $\mathbb{E}\big[\|\nabla\mathcal{E}_S^n\|^2\big]$.

$$\mathbb{E}\big[\|\nabla\mathcal{E}_S^n\|^2\big] = \mathbb{E}\Bigg[\Bigg(\frac{1}{J_l}\sum_{i=1}^{J_l}\big(\nabla\mathbb{E}[u_{i,l}^n]-\nabla u_{i,l}^n\big),\frac{1}{J_l}\sum_{j=1}^{J_l}\big(\nabla E[u_{j,l}^n]-\nabla u_{j,l}^n\big)\Bigg)\Bigg]$$

$$= \frac{1}{{J_l}^2}\sum_{i,j=1}^{J_l}\mathbb{E}\Bigg[\Bigg(\nabla\mathbb{E}[u_l^n]-\nabla u_{i,l}^n,\nabla\mathbb{E}[u_l^n]-\nabla u_{j,l}^n\Bigg)\Bigg]$$

$$= \frac{1}{{J_l}^2}\sum_{j=1}^{J_l}\mathbb{E}\Bigg[\Bigg(\nabla\mathbb{E}[u_l^n]-\nabla u_{j,l}^n,\nabla\mathbb{E}[u_l^n]-\nabla u_{j,l}^n\Bigg)\Bigg].$$

The last equality is due to the fact that $u_{1,l}^n,\dots,u_{J_l,l}^n$ are i.i.d., and thus the expected value of $\big(\nabla\mathbb{E}[u_l^n]-\nabla u_{i,l}^n,\nabla\mathbb{E}[u_l^n]-\nabla u_{j,l}^n\big)$ is a zero for $i\neq j$. We now expand $\mathbb{E}\big[\big(\nabla\mathbb{E}[u_l^n]-\nabla u_{j,l}^n,\nabla\mathbb{E}[u_l^n]-\nabla u_{j,l}^n\big)\big]$ and use the fact that $\mathbb{E}[\nabla u_{j,l}^n]=\nabla\mathbb{E}[u_{j,l}^n]$ and $\mathbb{E}[u_l^n]=\mathbb{E}[u_{j,l}^n]$ to obtain

$$\mathbb{E}\big[\|\nabla\mathcal{E}_S^n\|^2\big] = -\frac{1}{J_l}\|\nabla\mathbb{E}[u_{j,l}^n]\|^2+\frac{1}{J_l}\mathbb{E}[\|\nabla u_{j,l}^n\|^2],$$

which yields

$$\mathbb{E}\big[\|\nabla\mathcal{E}_S^n\|^2\big] \le \frac{1}{J_l}\mathbb{E}\big[\|\nabla u_{j,l}^n\|^2\big].$$

With the help pf Theorem 1, we have

$$\Big(\frac{\theta}{3}-\theta_+\Big)\Delta t_l\sum_{n=1}^{N_l}\mathbb{E}\big[\|\nabla\mathcal{E}_S^n\|^2\big] \le \frac{C}{J_l}\Big(\frac{\Delta t_l}{\theta-3\theta_+}\sum_{n=1}^{N_l}\mathbb{E}\big[\|f_j^n\|_{-1}^2\big] + \theta\Delta t_l\mathbb{E}\big[\|\nabla u_{j,l}^1\|^2+\|\nabla u_{j,l}^0\|^2\big]+\mathbb{E}\big[\|u_{j,l}^1\|^2+\|2u_{j,l}^1-u_{j,l}^0\|^2\big]\Big). \tag{19}$$

The other terms on the LHS of (18) can be treated in the same manner. This completes the proof. ∎

Next, we estimate the finite element discretization error $\mathcal{E}_l^n$.

THEOREM 4. *Let $\mathcal{E}_l^n=\mathbb{E}[u_j(t_n)-u_{j,l}^n]$, where $u_j(t_n)$ is the solution to equation (1) when $\omega=\omega_j$ and $t=t_n$ and $u_{j,l}^n$ is the result of scheme (4). Assume that the initial errors $\|u_j(t_0)-u_{j,l}^0\|$, $\|u_j(t_1)-u_{j,l}^1\|$, $\|\nabla(u_j(t_0)-u_{j,l}^0)\|$ and $\|\nabla(u_j(t_1)-u_{j,l}^1)\|$ are all at least $\mathcal{O}(h^m)$. Suppose conditions* (i) *and* (ii)*, and the stability condition (5) hold, there exists a generic constant C independent of J_l, h_l and Δt_l such that*

$$\frac{1}{4}\mathbb{E}\big[\|\mathcal{E}_l^{N_l}\|^2\big]+\frac{1}{4}\mathbb{E}\big[\|2\mathcal{E}_l^{N_l}-\mathcal{E}_l^{N_l-1}\|^2\big]+\Big(\frac{\theta}{3}-\theta_+\Big)\Delta t_l\sum_{n=1}^{N_l}\mathbb{E}\big[\|\nabla\mathcal{E}_l^n\|^2\big] \le C(\Delta t_l^4+h_l^{2m}). \tag{20}$$

Proof. We first derive the error equation for (4). Equation (1) evaluated at t_{n+1} and tested by $\forall\, v_l\in V_l^0$ yields

$$\left(\frac{3u_j(t_{n+1})-4u_j(t_n)+u_j(t_{n-1})}{2\Delta t_l},v_l\right)+(a_j\nabla u_j(t_{n+1}),\nabla v_l) = (f_j^{n+1},v_l)-(R_j^{n+1},v_l), \tag{21}$$

where $f_j^{n+1} = f_j(t_{n+1})$ and $R_j^{n+1} = u_{j,t}(t_{n+1}) - \frac{3u_j(t_{n+1})-4u_j(t_n)+u_j(t_{n-1})}{2\Delta t_l}$. Denoted by $e_j^n := u_j(t_n) - u_{j,l}^n$ the approximation error at the time t_n. Subtracting (4) from (21) produces

$$\left(\frac{3e_j^{n+1} - 4e_j^n + e_j^{n-1}}{2\Delta t_l}, v_l\right) + (\overline{a}_l \nabla e_j^{n+1}, \nabla v_l) + \big((a_j - \overline{a}_l)\nabla(2e_j^n - e_j^{n-1}), \nabla v_l\big) + \big((a_j - \overline{a}_l)\nabla(u_j^{n+1} - 2u_j^n + u_j^{n-1}), \nabla v_l\big) + (R_j^{n+1}, v_l) = 0. \tag{22}$$

Let $P_l(u_j(t_n))$ be the Ritz projection of $u_j(t_n)$ onto V_l^0 satisfying

$$\big(\overline{a}_l\big(\nabla(u_j(t_n) - P_l(u_j(t_n)))\big), \nabla v_l\big) = 0, \quad \forall\, v_l \in V_l^0.$$

The error can be decomposed as

$$e_j^n = \rho_{j,l}^n - \phi_{j,l}^n \text{ with } \rho_{j,l}^n = u_j(t_n) - P_l(u_j(t_n)) \text{ and } \phi_{j,l}^n = u_{j,l}^n - P_l(u_j(t_n)).$$

By substituting this decomposition into (22) and choosing $v_l = \phi_{j,l}^{n+1}$, we obtain

$$\begin{aligned}
&\left(\frac{3\phi_{j,l}^{n+1} - 4\phi_{j,l}^n + \phi_{j,l}^{n-1}}{2\Delta t_l}, \phi_{j,l}^{n+1}\right) + (\overline{a}_l \nabla \phi_{j,l}^{n+1}, \nabla \phi_{j,l}^{n+1}) \\
&\quad = -\Big((a_j - \overline{a}_l)\nabla(2\phi_{j,l}^n - \phi_{j,l}^{n-1}), \nabla \phi_{j,l}^{n+1}\Big) + \left(\frac{3\rho_{j,l}^{n+1} - 4\rho_{j,l}^n + \rho_{j,l}^{n-1}}{2\Delta t_l}, \phi_{j,l}^{n+1}\right) \\
&\quad + (\overline{a}_l \nabla \rho_{j,l}^{n+1}, \nabla \phi_{j,l}^{n+1}) + \Big((a_j - \overline{a}_l)\nabla(2\rho_{j,l}^n - \rho_{j,l}^{n-1}), \nabla \phi_{j,l}^{n+1}\Big) \\
&\quad + \Big((a_j - \overline{a}_l)\nabla(u_j^{n+1} - 2u_j^n + u_j^{n-1}), \nabla \phi_{j,l}^{n+1}\Big) + (R_j^{n+1}, \phi_{j,l}^{n+1}).
\end{aligned} \tag{23}$$

After integrating over probability space, we have, for the LHS,

$$\begin{aligned}
\text{LHS} \geq\ & \frac{1}{4\Delta t_l}\mathbb{E}\big[\|\phi_{j,l}^{n+1}\|^2 + \|2\phi_{j,l}^{n+1} - \phi_{j,l}^n\|^2\big] - \frac{1}{4\Delta t_l}\mathbb{E}\big[\|\phi_{j,l}^n\|^2 + \|2\phi_{j,l}^n - \phi_{j,l}^{n-1}\|^2\big] \\
& + \frac{1}{4\Delta t_l}\mathbb{E}\big[\|\phi_{j,l}^{n+1} - 2\phi_{j,l}^n + \phi_{j,l}^{n-1}\|^2\big] + \theta\mathbb{E}\big[\|\nabla \phi_{j,l}^{n+1}\|^2\big].
\end{aligned} \tag{24}$$

We then bound the terms on the RHS of (23) one by one. By applying the Cauchy-Schwarz and Young's inequalities, we have

$$\begin{aligned}
&\mathbb{E}\Big[\Big|\Big((a_j - \overline{a}_l)\nabla(2\phi_{j,l}^n - \phi_{j,l}^{n-1}), \nabla \phi_{j,l}^{n+1}\Big)\Big|\Big] \\
&\leq \theta_+\mathbb{E}\big[|(2\nabla\phi_{j,l}^n, \nabla\phi_{j,l}^{n+1})|\big] + \theta_+\mathbb{E}\big[|(\nabla\phi_{j,l}^{n-1}, \nabla\phi_{j,l}^{n+1})|\big] \\
&\leq \theta_+\mathbb{E}\big[\|\nabla\phi_{j,l}^n\|^2\big] + \frac{\theta_+}{2}\mathbb{E}\big[\|\nabla\phi_{j,l}^{n-1}\|^2\big] + \frac{3\theta_+}{2}\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big].
\end{aligned} \tag{25}$$

We further use the Poincáre inequality and have

$$
\begin{aligned}
(26)\quad & \mathbb{E}\left[\left|\left(\frac{3\rho_{j,l}^{n+1}-4\rho_j^n+\rho_{j,l}^{n-1}}{2\Delta t_l}, \phi_{j,l}^{n+1}\right)\right|\right] \\
& \le \frac{C}{4C_0\theta}\mathbb{E}\left[\left\|\frac{3\rho_{j,l}^{n+1}-4\rho_j^n+\rho_{j,l}^{n-1}}{2\Delta t_l}\right\|^2\right] + C_0\theta\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big] \\
& \le \frac{C}{4C_0\theta}\mathbb{E}\left[\left\|\frac{1}{\Delta t_l}\int_{t_{n-1}}^{t_{n+1}}\rho_{j,t}\,dt\right\|^2\right] + C_0\theta\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big] \\
(27)\quad & \le \frac{C}{4C_0\theta\Delta t_l}\mathbb{E}\left[\int_{t^{n-1}}^{t^{n+1}}\|\rho_{j,t}\|^2dt\right] + C_0\theta\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big],
\end{aligned}
$$

where C is the Poincáre coefficient and C_0 is an arbitrary positive constant. The rest of terms can be bounded as follows.

$$
(28)\quad \mathbb{E}\left[\left|(\overline{a}_l\nabla\rho_{j,l}^{n+1}, \nabla\phi_{j,l}^{n+1})\right|\right] = 0.
$$

$$
\begin{aligned}
(29)\quad & \mathbb{E}\left[\left|\Big((a_j-\overline{a}_l)\nabla(2\rho_{j,l}^n-\rho_j^{n-1}), \nabla\phi_{j,l}^{n+1}\Big)\right|\right] \\
& \le \theta_+\mathbb{E}\big[|(2\nabla\rho_{j,l}^n, \nabla\phi_{j,l}^{n+1})|\big] + \theta_+\mathbb{E}\big[|(\nabla\rho_j^{n-1}, \nabla\phi_{j,l}^{n+1})|\big] \\
& \le \frac{1}{C_0}\frac{\theta_+^2}{\theta}\mathbb{E}\big[\|\nabla\rho_j^n\|^2\big] + \frac{1}{4C_0}\frac{\theta_+^2}{\theta}\mathbb{E}\big[\|\nabla\rho_j^{n-1}\|^2\big] + 2C_0\theta\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big].
\end{aligned}
$$

$$
\begin{aligned}
(30)\quad & \mathbb{E}\left[\left|((a_j-\overline{a})\nabla(u_j^{n+1}-2u_j^n+u_j^{n-1}), \nabla\phi_{j,l}^{n+1})\right|\right] \\
& \le \frac{1}{4C_0}\frac{\theta_+^2}{\theta}\mathbb{E}\big[\|\nabla(u_j^{n+1}-2u_j^n+u_j^{n-1})\|^2\big] + C_0\theta\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big] \\
& \le \frac{C\Delta t_l^3}{4C_0}\frac{\theta_+^2}{\theta}\mathbb{E}\Big[\int_{t^{n-1}}^{t^{n+1}}\|\nabla u_{j,tt}\|^2dt\Big] + C_0\theta\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big],
\end{aligned}
$$

and

$$
(31)\quad \mathbb{E}\left[\left|(R_j^{n+1}, \phi_{j,l}^{n+1})\right|\right] \le C_0\theta\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big] + \frac{C\Delta t_l^3}{C_0\theta}\mathbb{E}\Big[\int_{t^{n-1}}^{t^{n+1}}\|u_{j,ttt}\|^2dt\Big].
$$

Substituting (24) to (31) into (23), we get

$$
\begin{aligned}
& \frac{1}{4\Delta t_l}\big(\mathbb{E}\big[\|\phi_{j,l}^{n+1}\|^2\big] + \mathbb{E}\big[\|2\phi_{j,l}^{n+1}-\phi_{j,l}^n\|^2\big]\big) - \frac{1}{4\Delta t_l}\big(\mathbb{E}\big[\|\phi_{j,l}^n\|^2\big] + \mathbb{E}\big[\|2\phi_{j,l}^n-\phi_{j,l}^{n-1}\|^2\big]\big) \\
& + \frac{1}{4\Delta t_l}\mathbb{E}\big[\|\phi_{j,l}^{n+1}-2\phi_{j,l}^n+\phi_{j,l}^{n-1}\|^2\big] + \theta(1-5C_0-\frac{3\theta_+}{2\theta})\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big] \\
& - \theta_+\mathbb{E}\big[\|\nabla\phi_{j,l}^n\|^2\big] - \frac{\theta_+}{2}\mathbb{E}\big[\|\nabla\phi_{j,l}^{n-1}\|^2\big] \\
& \le \frac{C}{4C_0\theta\Delta t_l}\mathbb{E}\left[\int_{t^{n-1}}^{t^{n+1}}\|\rho_{j,t}\|^2dt\right] + \frac{\theta_+^2}{C_0\theta}\mathbb{E}\big[\|\nabla\rho_j^n\|^2\big] + \frac{\theta_+^2}{4C_0\theta}\mathbb{E}\big[\|\nabla\rho_{j,l}^{n-1}\|^2\big] \\
& + \frac{C\Delta t_l^3}{4C_0}\frac{\theta_+^2}{\theta}\mathbb{E}\Big[\int_{t^{n-1}}^{t^{n+1}}\|\nabla u_{j,tt}\|^2dt\Big] + \frac{C\Delta t_l^3}{C_0\theta}\mathbb{E}\Big[\int_{t^{n-1}}^{t^{n+1}}\|u_{j,ttt}\|^2dt\Big].
\end{aligned}
$$

Now we split the term $\theta\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big]$, and choose $C_0 = \frac{1}{30}(1 - \frac{3\theta_+}{\theta})$:

(32)

$$\frac{1}{4\Delta t_l}(\mathbb{E}\big[\|\phi_{j,l}^{n+1}\|^2\big] + \mathbb{E}\big[\|2\phi_{j,l}^{n+1} - \phi_{j,l}^{n}\|^2\big]) - \frac{1}{4\Delta t}(\mathbb{E}\big[\|\phi_{j,l}^{n}\|^2\big] + \mathbb{E}\big[\|2\phi_{j,l}^{n} - \phi_{j,l}^{n-1}\|^2\big])$$
$$+ \frac{1}{4\Delta t_l}\mathbb{E}\big[\|\phi_{j,l}^{n+1} - 2\phi_{j,l}^{n} + \phi_{j,l}^{n-1}\|^2\big] + \theta\Big(\frac{1}{3} - \frac{\theta_+}{\theta}\Big)\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big]$$
$$+ \theta\Big(\frac{1}{3} - \frac{\theta_+}{\theta}\Big)\mathbb{E}\big[\|\nabla\phi_{j,l}^{n}\|^2\big] + \theta\Big(\frac{1}{6} - \frac{\theta_+}{2\theta}\Big)\mathbb{E}\big[\|\nabla\phi_{j,l}^{n-1}\|^2\big]$$
$$+ \frac{\theta}{2}\Big(\mathbb{E}\big[\|\nabla\phi_{j,l}^{n+1}\|^2\big] - \mathbb{E}\big[\|\nabla\phi_{j,l}^{n}\|^2\big]\Big) + \frac{\theta}{6}\Big(\mathbb{E}\big[\|\nabla\phi_{j,l}^{n}\|^2\big] - \mathbb{E}\big[\|\nabla\phi_{j,l}^{n-1}\|^2\big]\Big)$$
$$\leq \frac{C}{(\theta - 3\theta_+)}\Big\{\frac{1}{\Delta t_l}\mathbb{E}\left[\int_{t^{n-1}}^{t^{n+1}} \|\rho_{j,t}\|^2 dt\right] + \theta_+^2\mathbb{E}\big[\|\nabla\rho_j^n\|^2\big] + \theta_+^2\mathbb{E}\big[\|\nabla\rho_{j,l}^{n-1}\|^2\big]$$
$$+ C\Delta t_l^3\theta_+^2\mathbb{E}\Big[\int_{t^{n-1}}^{t^{n+1}} \|\nabla u_{j,tt}\|^2 dt\Big] + \Delta t_l^3\mathbb{E}\Big[\int_{t^{n-1}}^{t^{n+1}} \|u_{j,ttt}\|^2 dt\Big]\Big\}.$$

Summing (32) from $n = 1$ to $N_l - 1$, multiplying both sides by Δt_l, and dropping several positive terms, we have

(33)

$$\frac{1}{4}\mathbb{E}\big[\|\phi_{j,l}^{N_l}\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2\phi_{j,l}^{N_l} - \phi_{j,l}^{N_l-1}\|^2\big] + \Big(\frac{\theta}{3} - \theta_+\Big)\Delta t_l\sum_{n=1}^{N_l}\mathbb{E}\big[\|\nabla\phi_{j,l}^{n}\|^2\big]$$
$$\leq \frac{C}{(\theta - 3\theta_+)}\sum_{n=1}^{N_l-1}\left\{\mathbb{E}\left[\int_{t^{n-1}}^{t^{n+1}} \|\rho_{j,t}\|^2 dt\right] + \Delta t_l\theta_+^2\mathbb{E}\big[\|\nabla\rho_j^n\|^2\big] + \Delta t_l\theta_+^2\mathbb{E}\big[\|\nabla\rho_{j,l}^{n-1}\|^2\big]\right.$$
$$\left.+ \Delta t_l^4\theta_+^2\mathbb{E}\Big[\int_{t^{n-1}}^{t^{n+1}} \|\nabla u_{j,tt}\|^2 dt\Big] + \Delta t_l^4\mathbb{E}\Big[\int_{t^{n-1}}^{t^{n+1}} \|u_{j,ttt}\|^2 dt\Big]\right\}$$
$$+ \frac{1}{4}\mathbb{E}\big[\|\phi_{j,l}^{1}\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2\phi_{j,l}^{1} - \phi_{j,l}^{0}\|^2\big] + \frac{\theta}{2}\Delta t_l\mathbb{E}\big[\|\nabla\phi_{j,l}^{1}\|^2\big] + \frac{\theta}{6}\Delta t_l\mathbb{E}\big[\|\nabla\phi_{j,l}^{0}\|^2\big].$$

By the regularity assumption and standard finite element estimates of Ritz projection error (see, e.g., Lemma 13.1 in [39]), namely, for any $u_j^n \in H^{m+1}(D) \cap H_0^1(D)$,

$$\|\rho_{j,l}^n\|^2 \leq Ch_l^{2m+2}\|u_j(t_n)\|_{l+1}^2 \quad \text{and} \quad \|\nabla\rho_{j,l}^n\|^2 \leq Ch_l^{2m}\|u_j(t_n)\|_{l+1}^2, \tag{34}$$

and use the assumption that $\|e_{j,l}^0\|$, $\|e_{j,l}^1\|$, $\|\nabla e_{j,l}^0\|$, and $\|\nabla e_{j,l}^1\|$ are at least $\mathcal{O}(h^m)$, we have

$$\begin{aligned}
&\frac{1}{4}\mathbb{E}\big[\|\phi_{j,l}^{N_l}\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2\phi_{j,l}^{N_l} - \phi_{j,l}^{N_l-1}\|^2\big] + \Big(\frac{\theta}{3} - \theta_+\Big)\Delta t_l\sum_{n=1}^{N_l}\mathbb{E}\big[\|\nabla\phi_{j,l}^{n}\|^2\big]\\
&\leq \frac{C}{(\theta - 3\theta_+)}\Big\{h_l^{2m+2} + \theta_+^2h_l^{2m} + \Delta t_l^4\theta_+^2\mathbb{E}\Big[\int_0^T \|\nabla u_{j,tt}\|^2 dt\Big]\\
&+ \Delta t_l^4\mathbb{E}\Big[\int_0^T \|u_{j,ttt}\|^2 dt\Big]\Big\} + h_l^{2m} + \theta\Delta t_l h_l^{2m},
\end{aligned} \tag{35}$$

where C is a generic constant independent of the sample size J_l, time step Δt_l and mesh size h_l. By the triangle inequality, we have

$$\frac{1}{4}\mathbb{E}\big[\|u_j(t_{N_l}) - u_{j,l}^{N_l}\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2\big(u_j(t_{N_l}) - u_{j,l}^{N_l}\big) - \big(u_j(t_{N_l-1}) - u_{j,l}^{N_l-1}\big)\|^2\big] + \Big(\frac{\theta}{3} - \theta_+\Big)\Delta t_l \sum_{n=1}^{N_l} \mathbb{E}\big[\|\nabla\big(u_j(t_n - u_{j,l}^n\big)\|^2\big] \le C(\Delta t_l^4 + h_l^{2m}).$$

Applying Jensen's inequality to terms on the LHS leads to the error estimate (20). This completes the proof. ∎

The combination of the error contributions from the Monte Carlo sampling and finite element approximation leads to the following estimate for the l-th level Monte Carlo ensemble approximation.

THEOREM 5. *Let $u(t_n)$ be the solution to equation* (1) *and $\Psi_{J_l}^n = \frac{1}{J_l}\sum_{j=1}^{J_l} u_{j,l}^n$. Suppose conditions* (i) *and* (ii) *hold, and suppose the stability condition (5) is satisfied, then*

$$\begin{aligned}
&\frac{1}{4}\mathbb{E}\big[\|\mathbb{E}[u(t_{N_l})] - \Psi_{J_l}^{N_l}\|^2\big] + \frac{1}{4}\mathbb{E}\big[\|2(\mathbb{E}[u(t_{N_l})] - \Psi_{J_l}^{N_l}) - (\mathbb{E}[u(t_{N_l-1})] - \Psi_{J_l}^{N_l-1})\|^2\big] \\
&+ \Big(\frac{\theta}{3} - \theta_+\Big)\Delta t_l \sum_{n=1}^{N_l} \mathbb{E}[\|\nabla(\mathbb{E}[u(t_n)] - \Psi_{J_l}^n)\|^2] \\
&\le \frac{C}{J_l}\Big(\Delta t_l \sum_{n=1}^{N_l} \mathbb{E}\big[\|f_j^n\|_{-1}^2\big] + \Delta t_l \mathbb{E}\big[\|\nabla u_{j,l}^1\|^2 + \|\nabla u_{j,l}^0\|^2\big] \\
&+ \mathbb{E}\big[\|u_{j,l}^1\|^2 + \|2u_{j,l}^1 - u_{j,l}^0\|^2\big]\Big) + C(\Delta t_l^4 + h_l^{2m}),
\end{aligned} \tag{36}$$

where C is a positive constant independent of $J_l, \Delta t_l$ and h_l.

Proof. Consider the first term on the LHS of (36). By the triangle and Young's inequalities, we get

$$\mathbb{E}\big[\|\mathbb{E}[u(t_{N_l})] - \Psi_{J_l}^{N_l}\|^2\big] \le 2\big(\mathbb{E}\big[\|\mathbb{E}[u_j(t_{N_l})] - \mathbb{E}[u_{j,l}^{N_l}]\|^2\big] + \mathbb{E}\big[\|\mathbb{E}[u_{j,l}^{N_l}] - \Psi_{J_l}^{N_l}\|^2\big]\big).$$

Then the conclusion follows from Theorems 3-4. The other terms on the LHS of (36) can be estimated in the same manner. ∎

4.2. Multilevel Monte Carlo ensemble finite element method. Now, we derive the error estimate for the MLMCE method.

THEOREM 6. *Suppose conditions* (i) *and* (ii) *and the stability condition (5) hold, then the MLMCE approximation error satisfies*

$$\begin{aligned}
&\frac{1}{4}\mathbb{E}\left[\big\|\mathbb{E}\big[u(t_{N_L})\big] - \Psi\big[u_L(t_{N_L})\big]\big\|^2\right] + \frac{1}{4}\mathbb{E}\Big[\big\|\mathbb{E}\big[u^{N_L}\big] - \Psi\big[u_L(t_{N_L})\big] - \big(\mathbb{E}\big[u^{N_L-1}\big] \\
&- \Psi\big[u_L(t_{N_L-1})\big]\big)\big\|^2\Big] + \Big(\frac{\theta}{3} - \theta_+\Big)\Delta t_L \sum_{n=1}^{N_L} \mathbb{E}\Big[\big\|\nabla\mathbb{E}\big[u(t_n)\big] - \nabla\Psi\big[u_L(t_n)\big]\big\|^2\Big] \\
&\le C\Big(h_L^{2m} + \Delta t_L^4 + \sum_{l=1}^{L} \frac{1}{J_l}(h_l^{2m} + \Delta t_l^4)\Big) + \frac{C}{J_0}\Big(\Delta t_0 \sum_{n=1}^{N_0} \mathbb{E}\big[\|f_j^n\|_{-1}^2\big] \\
&+ \Delta t_0 \mathbb{E}\big[\|\nabla u_{j,0}^1\|^2 + \|\nabla u_{j,0}^0\|^2\big] + \mathbb{E}\big[\|u_{j,0}^1\|^2 + \|2u_{j,0}^1 - u_{j,0}^0\|^2\big]\Big),
\end{aligned} \tag{37}$$

where $C > 0$ is a constant independent of $J_l, \Delta t_l$ and h_l.

Proof. We only analyze the first term on the LHS because the other terms can be treated in the same manner. First, we introduce $u_{-1}(t) = 0$.

$$\begin{aligned}
&\mathbb{E}\left[\left\|\mathbb{E}[u(t_{N_L})] - \Psi[u_L(t_{N_L})]\right\|^2\right] \\
&= \mathbb{E}\Big[\Big\|\mathbb{E}[u(t_{N_L})] - \mathbb{E}[u_L(t_{N_L})] + \mathbb{E}[u_L(t_{N_L})] - \sum_{l=0}^{L} \Psi_{J_l}[u_l(t_{N_L}) - u_{l-1}(t_{N_L})]\Big\|^2\Big] \\
&\le C\Bigg(\mathbb{E}\Big[\Big\|\mathbb{E}[u(t_{N_L})] - \mathbb{E}[u_L(t_{N_L})]\Big\|^2\Big] + \sum_{l=0}^{L} \mathbb{E}\Big[\Big\|\Big(\mathbb{E}[u_l(t_{N_L}) - u_{l-1}(t_{N_L})] \\
&\qquad - \Psi_{J_l}[u_l(t_{N_L}) - u_{l-1}(t_{N_L})]\Big)\Big\|^2\Big]\Bigg).
\end{aligned} \tag{38}$$

By Jensen's inequality and Theorem 4, we get

$$\begin{aligned}
\mathbb{E}\Big[\Big\|\mathbb{E}[u(t_{N_L})] - \mathbb{E}[u_L(t_{N_L})]\Big\|^2\Big] &\le \mathbb{E}\Big[\Big\|u(t_{N_L}) - u_L(t_{N_L})\Big\|^2\Big] \\
&\le C(\Delta t_L^4 + h_L^{2m}).
\end{aligned} \tag{39}$$

By Theorems 3-4 and the triangle inequality, we have

$$\begin{aligned}
&\mathbb{E}\Big[\Big\|\mathbb{E}[u_l(t_{N_L}) - u_{l-1}(t_{N_L})] - \Psi_{J_l}[u_l(t_{N_L}) - u_{l-1}(t_{N_L})]\Big\|^2\Big] \\
&= \mathbb{E}\Big[\Big\|(\mathbb{E} - \Psi_{J_l})[u_l(t_{N_L}) - u_{l-1}(t_{N_L})]\Big\|^2\Big] \\
&\le \frac{1}{J_l}\mathbb{E}\big[\|u_l(t_{N_L}) - u_{l-1}(t_{N_L})\|^2\big] \\
&\le \frac{2}{J_l}\Big(\mathbb{E}\big[\|u(t_{N_L}) - u_l(t_{N_L})\|^2\big] + \mathbb{E}\big[\|u(t_{N_L}) - u_{l-1}(t_{N_L})\|^2\big]\Big) \\
&\le \frac{C}{J_l}\big(\Delta t_l^4 + h_l^{2m} + \Delta t_{l-1}^4 + h_{l-1}^{2m}\big) \le \frac{C}{J_l}\big(\Delta t_l^4 + h_l^{2m}\big).
\end{aligned} \tag{40}$$

Meanwhile, based on Theorem 5, we have

$$\begin{aligned}
&\mathbb{E}\big[\|\mathbb{E}[u_0(t_{N_L})] - \Psi_{J_0}[u_0(t_{N_L})]\|^2\big] \\
&\le \frac{C}{J_0}\Big(\Delta t_0 \sum_{n=1}^{N_0} \mathbb{E}\big[\|f_j^n\|_{-1}^2\big] + \Delta t_0 \mathbb{E}\big[\|\nabla u_{j,0}^1\| + \|\nabla u_{j,0}^0\|^2\big] \\
&\quad + \mathbb{E}\big[\|u_{j,0}^1\|^2 + \|2u_{j,0}^1 - u_{j,0}^0\|^2\big]\Big).
\end{aligned} \tag{41}$$

Plugging (39), (40) and (41) into (38), we have

$$\begin{aligned}
&\frac{1}{4}\mathbb{E}\big[\|\mathbb{E}[u(t_{N_L})] - \Psi[u_L(t_{N_L})]\|^2\big] \le C\Big(\Delta t_L^4 + h_L^{2m} + \sum_{l=1}^{L} \frac{1}{J_l}(\Delta t_l^4 + h_l^{2m})\Big) \\
&+ \frac{C}{J_0}\Big(\Delta t_0 \sum_{n=1}^{N_0} \mathbb{E}\big[\|f_j^n\|_{-1}^2\big] + \Delta t_0 \mathbb{E}\big[\|\nabla u_{j,0}^1\|^2 + \|\nabla u_{j,0}^0\|^2\big] \\
&+ \mathbb{E}\big[\|u_{j,0}^1\|^2 + \|2u_{j,0}^1 - u_{j,0}^0\|^2\big]\Big).
\end{aligned} \tag{42}$$

The other terms on the LHS of (37) can be treated in the same manner. This completes the proof. ∎

Since, in general, the finite element simulation cost increases as the mesh is refined, we can balance the time step size Δt_l, mesh size h_l and sampling size J_l in the preceding error estimation for achieving an optimal rate of convergence.

Corollary 7. *By taking*

$$\Delta t_l = \mathcal{O}\big(\sqrt{h_l^m}\big) \quad \text{and} \quad J_l = \mathcal{O}\big(l^{1+\varepsilon} 2^{2m(L-l)}\big)$$

for an arbitrarily small positive constant ϵ and $l = 0, 1, \cdots, L$, the MLMCE approximation satisfies

$$\begin{aligned}(43)\quad &\frac{1}{4}\mathbb{E}\left[\big\|\mathbb{E}\big[u(t_{N_L})\big] - \Psi\big[u_L(t_{N_L})\big]\big\|^2\right] + \frac{1}{4}\mathbb{E}\Big[\big\|\mathbb{E}\big[u^{N_L}\big] - \Psi\big[u_L(t_{N_L})\big] - \big(\mathbb{E}\big[u^{N_L-1}\big] \\ &- \Psi\big[u_L(t_{N_L-1})\big]\big)\big\|^2\Big] + \Big(\frac{\theta}{3} - \theta_+\Big)\Delta t_L \sum_{n=1}^{N_L} \mathbb{E}\Big[\big\|\nabla\mathbb{E}\big[u(t_n)\big] - \nabla\Psi\big[u_L(t_n)\big]\big\|^2\Big] \\ &\le C h_L^{2m},\end{aligned}$$

where $C > 0$ are constants independent of $J_l, \Delta t_l$ and h_l.

Similar to the MLMC method [7, 38, 16], one can choose the sample size in MLMCE by minimizing the total computational cost while achieving a desired error. Take $\Delta t_l = \mathcal{O}\big(\sqrt{h_l^m}\big)$ to match the spatial and temporal errors, and suppose that, as the mesh size decreases, the average cost of solving the PDE at level l increases and the average variance decreases in the following relations:

$$C_l = C h_l^{-\gamma_1} \text{ and } \sigma_l = C_\sigma h_l^{\beta},$$

where C, C_σ, γ_1 and β are some positive constants. One can optimize the number of samples at the l-th level, J_l, by minimizing the total sampling cost while ensuring the statistical error stays at the user-defined tolerance ϵ. This can be formulated as an unconstrained optimization problem using the Lagrangian approach:

$$\min_{J_l} \sum_{l=0}^{L} J_l C_l + \lambda \left[(L+1)\sum_{l=0}^{L} \frac{\sigma_l}{J_l} - \frac{\epsilon^2}{4}\right].$$

Applying the Euler-Lagrange condition, we get

$$J_l = \frac{4(L+1)}{\epsilon^2}\left(\sum_{l=0}^{L}\sqrt{\sigma_l C_l}\right)\sqrt{\frac{\sigma_l}{C_l}}$$

and the associated total cost is

$$C = \frac{4(L+1)}{\epsilon^2}\left(\sum_{l=0}^{L}\sqrt{\sigma_l C_l}\right)^2.$$

Note that, in this setting, the MLMCE shares the same expression of optimal sample size and total cost as those of the MLMC. However, the use of scheme (4) in MLMCE leads to smaller average cost for solving the PDE than the MLMC. Denote the average cost of MLMC at level l to be $C h_l^{-\gamma_2}$, we have $\gamma_1 < \gamma_2$ when either direct or block iterative methods are used in the linear solver. Let C^{MLMCE} and C^{MLMC} be the total costs of MLMCE and MLMC methods, respectively, we have

$$\frac{C^{MLMCE}}{C^{MLMC}} = \left(\frac{\sum_{l=0}^{L} \sqrt{\sigma_l h_l^{-\gamma_1}}}{\sum_{l=0}^{L} \sqrt{\sigma_l h_l^{-\gamma_2}}} \right)^2 = \left(\frac{\sum_{l=0}^{L} \sqrt{h_l^{\beta-\gamma_1}}}{\sum_{l=0}^{L} \sqrt{h_l^{\beta-\gamma_2}}} \right)^2 .$$

Then

$$\frac{C^{MLMCE}}{C^{MLMC}} = \begin{cases} h_0^{\beta-\gamma_1}/h_0^{\beta-\gamma_2} = h_0^{\gamma_2-\gamma_1} & \text{if } \gamma_2 < \beta, \\ h_0^{\beta-\gamma_1}/h_L^{\beta-\gamma_2} = 2^{L(\beta-\gamma_2)} h_0^{\gamma_2-\gamma_1} & \text{if } \gamma_1 < \beta < \gamma_2, \\ h_L^{\beta-\gamma_1}/h_L^{\beta-\gamma_2} = h_L^{\gamma_2-\gamma_1} & \text{if } \gamma_2 < \beta. \end{cases}$$

It is seen the total computational complexity of the MLMCE is lower than standard MLMC in any case. In particular, when the standard LU factorization is used in the linear solver, we can derive a more concrete computational complexity. Let d be the dimension of domain. The complexity for LU factorization is Ch^{-3d} and that for solving triangular systems is Ch^{-2d}. Then the total computational cost for sampling is $\sum_{l=0}^{L} \left(J_l h_l^{-2d} + h_l^{-3d} \right)$ since only one LU factorization is needed at each level. The corresponding optimal sample size is

$$J_l = \frac{4(L+1)}{\epsilon^2} \left(\sum_{l=0}^{L} \sqrt{\sigma_l h_l^{-2d}} \right) \sqrt{\sigma_l h_l^{2d}} \tag{44}$$

by minimizing the total cost while achieving error ϵ. The associated computational complexity is

$$C^{MLMCE} = \frac{4(L+1)}{\epsilon^2} \left(\sum_{l=0}^{L} \sqrt{\sigma_l h_l^{-2d}} \right)^2 + \sum_{l=0}^{L} h_l^{-3d}. \tag{45}$$

That of the optimized MLMC complexity is

$$C^{MLMC} = \frac{4(L+1)}{\epsilon^2} \left(\sum_{l=0}^{L} \sqrt{\sigma_l \left(h_l^{-2d} + h_l^{-3d} \right)} \right)^2 . \tag{46}$$

5. Numerical Experiments.

In this section, we apply the proposed ensemble-based multilevel Monte Carlo algorithm to two numerical tests for solving the random parabolic equation (1). The goal is two-fold: to illustrate the theoretical results in Test 1; and to show the efficiency of the proposed method in Test 2.

5.1. Test 1.

We first check the convergence rate of the MLMCE method numerically by considering a problem with an *a priori* known exact solution. The diffusion coefficient and the exact solution of equation (1) are selected as follows.

$$\begin{aligned} a(\omega, \mathbf{x}) &= 8 + (1+\omega)\sin(xy), \\ u(\omega, \mathbf{x}, t) &= (1+\omega)[\sin(2\pi x)\sin(2\pi y) + \sin(4\pi t)], \end{aligned}$$

where ω obeys a uniform distribution on $[-\sqrt{3}, \sqrt{3}]$, $t \in [0,1]$, and $(x,y) \in [0,1]^2$. The initial condition, inhomogeneous Dirichlet boundary condition and source term are chosen to match the prescribed exact solution. Therefore, the expectation of the solution is

$$\mathbb{E}[u] = \sin(2\pi x)\sin(2\pi y) + \sin(4\pi t).$$

For the spatial discretization, we use quadratic finite elements on uniform triangulations, that is, $m = 2$. To verify the analysis given in (7), we fix L and choose the mesh size $h_l = \sqrt{2}\cdot 2^{-2-l}$, time step size $\Delta t_l = 2^{-3-l}$, and number of samples $J_l = 2^{4(L-l)+1}$ at the l-th level of the MLMCE simulation for $l = 0, \ldots, L$. The experiment is repeated for $R = 10$ times. Let

$$\mathcal{E}_{L^2} = \sqrt{\frac{1}{R}\sum_{r=1}^{R}\left\|\mathbb{E}\big[u(T)\big] - \Psi\big[u_L^{(r)}(t_{N_L})\big]\right\|^2},$$

$$\mathcal{E}_{H^1} = \sqrt{\frac{1}{RM}\sum_{r=1}^{R}\sum_{m=1}^{M}\left\|\mathbb{E}\big[\nabla u(t_m)\big] - \Psi\big[\nabla u_L^{(r)}(t_m)\big]\right\|^2},$$

where u is the exact solution and $u_L^{(r)}$ is the MLMCE solution of the r-th replica. Hence, $\mathcal{E}_{L^2}$ and $\mathcal{E}_{H^1}$ represent the numerical error in L^2 and H^1 norms, respectively. With the above choice of discretization and sampling strategy, we expect both quantities converge quadratically with respect to h_L as indicated in Corollary 7 .

Table 1: Numerical errors of the MLMCE.

L	$\mathcal{E}_{L^2}$	rate	$\mathcal{E}_{H^1}$	rate
1	6.11×10^{-2}	-	5.60×10^{-1}	-
2	1.43×10^{-2}	2.10	1.50×10^{-1}	1.90
3	3.60×10^{-3}	1.99	3.81×10^{-2}	1.98

The MLMCE numerical errors as L varies from 1 to 3 are listed in Table 1. It is observed that both $\mathcal{E}_{L^2}$ and $\mathcal{E}_{H^1}$ converge at the order of nearly 2 with respect to h_L, which matches our expectation.

5.2. Test 2. Next, we use a test problem to demonstrate the effectiveness of the MLMCE method. The same test problem was considered in [26] for testing the first-order, ensemble-based Monte Carlo method and a similar computational setting was used in [30] to compare numerical approaches for parabolic equations with random coefficients.

The test problem is associated with the zero forcing term f, zero initial conditions, and homogeneous Dirichlet boundary conditions on the top, bottom and right edges of the domain but inhomogeneous Dirichlet boundary condition, $u = y(1-y)$, on the left edge. The random coefficient varies in the vertical direction and has the following form

$$a(\omega,\mathbf{x}) = a_0 + \sigma\sqrt{\lambda_0}Y_0(\omega) + \sum_{i=1}^{n_f}\sigma\sqrt{\lambda_i}\left[Y_i(\omega)\cos(i\pi y) + Y_{n_f+i}(\omega)\sin(i\pi y)\right] \tag{47}$$

with $\lambda_0 = \frac{\sqrt{\pi}L_c}{2}$, $\lambda_i = \sqrt{\pi}L_c e^{-\frac{(i\pi L_c)^2}{4}}$ for $i = 1, \ldots, n_f$ and $Y_0, \ldots, Y_{2n_f}$ are uncorrelated random variables with zero mean and unit variance. In the following numerical test, we take $a_0 = 1$, $L_c = 0.25$, $\sigma = 0.15$, $n_f = 3$ and assume the random variables $Y_0, \dots, Y_{2n_f}$ are independent and uniformly distributed in the interval $[-\sqrt{3}, \sqrt{3}]$. We use quadratic finite elements for spatial discretization and simulate the system over the time interval $[0, 0.5]$.

We use the MLMCE method to analyze some stochastic information of the system such as the expectation of the solution at final time. More precisely, we apply the MLMCE with the maximum level $L = 2$, the mesh size $h_l = \sqrt{2} \cdot 2^{-3-l}$ and time step size $\Delta t_l = 2^{-4-l}$. Due to the small size of the problem, we apply LU factorization in solving linear systems. Targeting a numerical error $\epsilon = 10^{-3}$, we choose the number of samples $J_l = 2^{4(L-l)+1}$ at the l-th level, for $l = 0, \dots, L$ based on (44) with $d = 2$ and $\beta = 4$. Note that if the samples does not satisfy the stability condition (5), we will divide the sample set into small subsets so that (5) holds on each smaller group. Since the diffusion coefficient function is independent of time, such a process can be efficiently implemented for ensemble calculations at each level. The MLMCE solution at the final time T is

$$\Psi_h^E(\mathbf{x}) = \Psi[u_L^E(t_{N_L})],$$

which is shown in Figure 1 (left).

Since the exact solution is unknown, to quantify the performance of the MLMCE method, we compare the result with that of the standard MLMC finite element simulations using the same computational setting. The same set of sample values is used, thus, the only difference is that individual finite element simulations are implemented at each level in the latter. Denote the approximated expected value of the latter

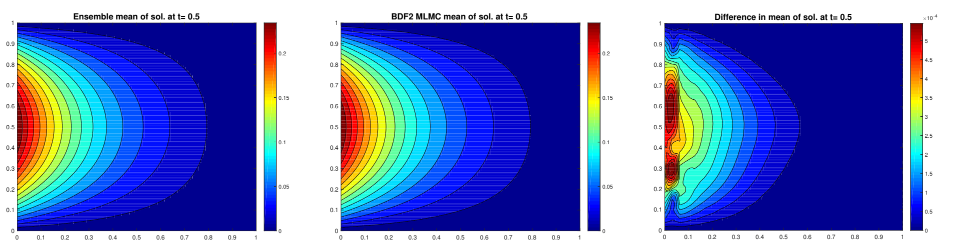

Fig. 1: Comparison of the simulation mean: MLMCE simulations (left), MLMC finite element simulations (middle), and the associated difference (right).

approach by

$$\Psi_h^I(\mathbf{x}) = \Psi[u_L^I(t_{N_L})],$$

which is shown in Figure 1 (middle). Note that for a fair comparison, we also use the LU factorization in solving all the linear systems in individual simulations. The difference between Ψ_h^E and Ψ_h^I, $|\Psi_h^E - \Psi_h^I|$, is shown in Figure 1 (right). It is observed that the difference is on the order of 10^{-4}, which indicates the MLMCE method is able to provide the same accurate approximation as individual simulations. However, the computational complexity of the MLMCE simulation is smaller than that of the individual MLMC simulations. By (45)-(46), we have the complexity estimations of both approaches as follows:

$$C^{MLMCE} = \frac{4(L+1)^3}{\epsilon^2} + \sum_{l=0}^{2} h_l^{-6} \approx 1.39 \times 10^9$$

and

$$C^{MLMC} = \frac{4(L+1)}{\epsilon^2}\left(\sum_{l=0}^{2} h_l^{-1}\right) \approx 5.37 \times 10^9.$$

Meanwhile, the CPU time for the ensemble simulation in this numerical test is 2.65×10^3 seconds and that of the MLMC finite element simulations is 1.01×10^4 seconds, which matches our complexity estimations.

6. Conclusions.

A multilevel Monte Carlo ensemble method is developed in this paper to solve second-order random parabolic partial differential equations. This method naturally combines the ensemble-based, multilevel Monte Carlo sampling approach with a second-order, ensemble-based time stepping scheme so that the computational efficiency for seeking stochastic solutions is improved. Numerical analysis shows the numerical approximation achieves the optimal order of convergence. As a next step, we will investigate performance of the method on large-scale, nonlinear problems, in which we will deal with nonlinearity of the system and use block iterative solvers to treat high-dimensional linear systems.

REFERENCES

[1] K. Ahuja, M. L. Parks, E. T. Phipps, A. G. SALINGER, and E. de Sturler, *Krylov recycling for climate modeling and uncertainty quantification*, CSRI Summer Proceedings, (2010), pp. 103–111.

[2] I. Babuška, F. Nobile, and R. Tempone, *A stochastic collocation method for elliptic partial differential equations with random input data*, SIAM Journal on Numerical Analysis, 45 (2007), pp. 1005–1034.

[3] I. Babuska, R. Tempone, and G. E. Zouraris, *Galerkin finite element approximations of stochastic elliptic partial differential equations*, SIAM Journal on Numerical Analysis, 42 (2004), pp. 800–825.

[4] A. Barth, C. Schwab, and N. Zollinger, *Multi-level Monte Carlo finite element method for elliptic PDEs with stochastic coefficients*, Numerische Mathematik, 119 (2011), pp. 123–161.

[5] J. Charrier, R. Scheichl, and A. L. Teckentrup, *Finite element error analysis of elliptic PDEs with random coefficients and its application to multilevel Monte Carlo methods*, SIAM Journal on Numerical Analysis, 51 (2013), pp. 322–352.

[6] A. T. Chronopoulos and A. B. Kucherov, *Block s-step Krylov iterative methods*, Numerical Linear Algebra with Applications, 17 (2010), pp. 3–15.

[7] K. A. Cliffe, M. B. Giles, R. Scheichl, and A. L. Teckentrup, *Multilevel Monte Carlo methods and applications to elliptic PDEs with random coefficients*, Computing and Visualization in Science, 14 (2011), pp. 3–15.

[8] Q. Du, V. Faber, and M. Gunzburger, *Centroidal Voronoi tessellations: Applications and algorithms*, SIAM Review, 41 (1999), pp. 637–676.

[9] J. A. Fiordilino, *Ensemble timestepping algorithms for the heat equation with uncertain conductivity*, arXiv preprint arXiv:1708.00893, (2017).

[10] M. Giles, *Improved multilevel Monte Carlo convergence using the Milstein scheme*, Monte Carlo and quasi-Monte Carlo methods 2006, (2008), pp. 343–358.

[11] M. B. Giles, *Multilevel Monte Carlo path simulation*, Operations Research, 56 (2008), pp. 607–617.

[12] M. Gunzburger, N. Jiang, and M. Schneier, *An ensemble-proper orthogonal decomposition method for the nonstationary Navier–Stokes equations*, SIAM Journal on Numerical Analysis, 55 (2017), pp. 286–304.

[13] M. Gunzburger, N. Jiang, and M. Schneier, *A higher-order ensemble/proper orthogonal decomposition method for the nonstationary Navier–Stokes equations*, (in press).

[14] M. Gunzburger, N. Jiang, and Z. Wang, *An efficient algorithm for simulating ensembles of parameterized flow problems*, IMA Journal of Numerical Analysis, DOI: https://doi.org/10.1093/imanum/dry029, (in press).

[15] M. Gunzburger, N. Jiang, and Z. Wang, *A second-order time-stepping scheme for simulating ensembles of parameterized flow problems*, Computational Methods in Applied Mathematics, DOI: https://doi.org/10.1515/cmam-2017-0051, (in press).

[16] M. D. Gunzburger, C. G. Webster, and G. Zhang, *Stochastic finite element methods for partial differential equations with random input data*, Acta Numerica, 23 (2014), pp. 521–650.

[17] M. H. Gutknecht, *Block Krylov space methods for linear systems with multiple right-hand sides: an introduction*, in: Modern Mathematical Models, Methods and Algorithms for Real World Systems, (2006).

[18] S. Heinrich, *Multilevel Monte Carlo methods, volume 2179 of lecture notes in computer science*, (2001), pp. 58–67.

[19] J. C. Helton and F. J. Davis, *Latin hypercube sampling and the propagation of uncertainty in analyses of complex systems*, Reliability Engineering & System Safety, 81 (2003), pp. 23–69.

[20] N. Jiang, *A higher order ensemble simulation algorithm for fluid flows*, Journal of Scientific Computing, 64 (2015), pp. 264–288.

[21] N. Jiang, *A second-order ensemble method based on a blended backward differentiation formula time-stepping scheme for time-dependent Navier–Stokes equations*, Numerical Methods for Partial Differential Equations, 33 (2017), pp. 34–61.

[22] N. Jiang, S. Kaya, and W. Layton, *Analysis of model variance for ensemble based turbulence modeling*, Computational Methods in Applied Mathematics, 15 (2015), pp. 173–188.

[23] N. Jiang and W. Layton, *An algorithm for fast calculation of flow ensembles*, International Journal for Uncertainty Quantification, 4 (2014), pp. 273–301.

[24] N. Jiang and W. Layton, *Numerical analysis of two ensemble eddy viscosity numerical regularizations of fluid motion*, Numerical Methods for Partial Differential Equations, 31 (2015), pp. 630–651.

[25] K. Liu and B. M. Rivière, *Discontinuous Galerkin methods for elliptic partial differential equations with random coefficients*, International Journal of Computer Mathematics, 90 (2013), pp. 2477–2490.

[26] Y. Luo and Z. Wang, *An ensemble algorithm for numerical solutions to deterministic and random parabolic PDEs*, SIAM Journal on Numerical Analysis, 56 (2018), pp. 859–876.

[27] J. Meng, P.-Y. Zhu, and H.-B. Li, *A block method for linear systems with multiple right-hand sides*, Journal of Computational and Applied Mathematics, 255 (2014), pp. 544–554.

[28] M. Mohebujjaman and L. G. Rebholz, *An efficient algorithm for computation of MHD flow ensembles*, Computational Methods in Applied Mathematics, 17 (2017), pp. 121–137.

[29] H. Niederreiter, *Random number generation and quasi-Monte Carlo methods*, vol. 63, SIAM, 1992.

[30] F. Nobile and R. Tempone, *Analysis and implementation issues for the numerical approximation of parabolic equations with random coefficients*, International journal for numerical methods in engineering, 80 (2009), pp. 979–1006.

[31] D. P. O'Leary, *The block conjugate gradient algorithm and related methods*, Linear algebra and its applications, 29 (1980), pp. 293–322.

[32] D. P. O'Leary, *Parallel implementation of the block conjugate gradient algorithm*, Parallel Computing, 5 (1987), pp. 127–139.

[33] M. L. Parks, E. De Sturler, G. Mackey, D. D. Johnson, and S. Maiti, *Recycling Krylov subspaces for sequences of linear systems*, SIAM Journal on Scientific Computing, 28 (2006), pp. 1651–1674.

[34] M. L. Parks, K. M. Soodhalter, and D. B. Szyld, *A block recycled GMRES method with investigations into aspects of solver performance*, arXiv preprint arXiv:1604.01713, (2016).

[35] V. J. Romero, J. V. Burkardt, M. D. Gunzburger, and J. S. Peterson, *Comparison of pure and Latinized centroidal Voronoi tessellation against various other statistical sampling methods*, Reliability Engineering & System Safety, 91 (2006), pp. 1266–1280.

[36] V. Simoncini and E. Gallopoulos, *Convergence properties of block GMRES and matrix polynomials*, Linear Algebra and its Applications, 247 (1996), pp. 97–119.

[37] A. Takhirov, M. Neda, and J. Waters, *Time relaxation algorithm for flow ensembles*, Numerical Methods for Partial Differential Equations, 32 (2016), pp. 757–777.

[38] A. L. Teckentrup, P. Jantsch, C. G. Webster, and M. Gunzburger, *A multilevel stochastic collocation method for partial differential equations with random input data*, SIAM/ASA Journal on Uncertainty Quantification, 3 (2015), pp. 1046–1074.

[39] V. Thomée, *Galerkin Finite Element Methods for Parabolic Problems*, vol. 1054, Springer Verlag, 1984.

[40] D. Xiu, *Fast numerical methods for stochastic computations: a review*, Communications in computational physics, 5 (2009), pp. 242–272.

[41] D. Xiu and G. E. Karniadakis, *A new stochastic approach to transient heat conduction modeling with uncertainty*, International Journal of Heat and Mass Transfer, 46 (2003), pp. 4681–4693.