INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 16, Number 2, Pages 225–239

A SECOND-ORDER CRANK-NICOLSON METHOD FOR TIME-FRACTIONAL PDES

MAX GUNZBURGER AND JILU WANG

Abstract. Based on convolution quadrature in time and continuous piecewise linear finite element approximation in space, a Crank-Nicolson type method is proposed for solving a partial differential equation involving a fractional time derivative. The method achieves second-order convergence in time without being corrected at the initial steps. Optimal-order error estimates are derived under regularity assumptions on the source and initial data but without having to assume regularity of the solution.

Key words. Crank-Nicolson scheme, time-fractional equation, convolution quadrature, finite element method, error estimates.

1. Introduction

Let $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$, denote a convex polygonal/polyhedral domain with boundary $\partial\Omega$, and consider the problem

$$(1)\qquad \begin{cases} \partial_t u(x,t) - \Delta\partial_t^{1-\alpha} u(x,t) = f(x,t) & (x,t) \in \Omega \times \mathbb{R}_+, \\ \partial_t^{1-\alpha} u(x,t) = 0 & (x,t) \in \partial\Omega \times \mathbb{R}_+, \\ u(x,0) = v(x) & x \in \Omega, \end{cases}$$

where $f(x,t)$ denotes a given source function and $v(x)$ given initial condition. The operator $\Delta : D(\Delta) \to L^2(\Omega)$ denotes the Laplacian, defined on the domain $D(\Delta) = \{\phi \in H_0^1(\Omega) : \Delta\phi \in L^2(\Omega)\}$, and $\partial_t^{1-\alpha} u$ denotes the left-sided Caputo fractional time derivative of order $1 - \alpha \in (0, 1)$, defined by (c.f. [11, pp. 91])

$$(2)\qquad \partial_t^{1-\alpha} u(x,t) := \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} \frac{\partial u(x,s)}{\partial s} \mathrm{d}s,$$

where $\Gamma(s) := \int_0^\infty t^{s-1} e^{-t} \mathrm{d}t$ denotes the Euler gamma function. We refer interested readers to [15, 21] for the regularity of solutions to (1) and its applications.

A number of numerical methods have been developed in the literature for solving PDE problems involving a fractional time derivative [3, 7, 12, 13, 14, 16, 19], among which the use of convolution quadrature (CQ) [12, 13] becomes more and more popular due to its excellent stability property and ease of implementation.

One of the main difficulties encountered when solving fractional evolution PDEs such as (1) is the low regularity of the solution in time (even with smooth initial data), which causes severe reduction of the convergence rates of high-order numerical schemes. In [3], Cuesta et al. overcame this difficulty by correcting the numerical scheme at the starting time step, which yielded second-order convergence of the numerical solutions based on certain regularity assumptions on the source and initial data. This idea was extended to the case $0 < \alpha < 1$ in [7] and [9], where second-order BDF and Crank-Nicolson type methods were proposed, respectively, for solving an equivalent formulation of (1). The schemes generally yield first-order

Received by the editors October 1, 2017 and, accepted October 24, 2017.
2000 *Mathematics Subject Classification.* 35R11, 26A33, 33F05.

convergence of the numerical solutions, but can be restored to second-order by correcting the schemes at several starting time steps. Of course, if a non-uniform mesh is used for time discretization, then the second-order convergence can be achieved without correction at the starting steps [16].

The models considered in [3, 7, 9, 16] are closely connected to (1), but they have different smoothing properties. As a result, the numerical schemes proposed in these previous works can not be applied directly to problem (1). In this paper, we develop a Crank-Nicolson scheme for problem (1) based on CQ in time and a continuous piecewise linear finite element method (FEM) in space. Inspired by [9], we combine the backward Euler CQ with a θ-type method for approximating $\Delta\partial_t^{1-\alpha}u$, and use the standard backward Euler method for approximating $\partial_t u$. Unlike [9], which approximates the equation at $t = t_n - \frac{\alpha\tau}{2}$, our method approximates the equation at $t = t_n - \frac{\tau}{2}$. The numerical method proposed in this paper is the only existing second-order method for (1) that does not require correction at the starting time steps.

For given initial data $v \in L^2(\Omega)$ and source $f \in W^{2,1}(0,T;L^2(\Omega))$, we prove the following error estimate:

$$\|u_h(t_n) - U_h^n\| \le C\tau^2\left(t_n^{-1}\|f(0)\| + \|f'(0)\| + \int_0^{t_n}\|f''(s)\|\mathrm{d}s\right), \tag{3}$$

where u_h and U_h^n denote the semidiscrete and fully discrete Galerkin finite element solutions, respectively. Here and below, for simplicity, we denote $u_h(t)$ and $f(t)$ by $u_h(x,t)$ and $f(x,t)$, respectively. The theoretical analysis is based on integral representations of u_h and U_h^n obtained by means of Laplace transform and generating function, a technique originating in [12, 13] and which proved to be powerful in [3, 8, 10, 9, 14, 17]. Numerical examples are presented to illustrate the convergence rate of the proposed method.

The rest of the paper is organized as follows. In Section 2, we present the fully discrete Crank-Nicolson Galerkin FEM for time-fractional PDE (1) and then state our main theoretical results. In Section 3, we prove optimal convergence rate for the approximate solution in time by using its integral representation and estimates of the resolvent operator. Numerical results are given in Section 4 to illustrate the theoretical analyses. Throughout this paper, we denote by C, with/without a subscript, a generic constant independent of h, n, and τ, which could be different at different occurrences.

2. The main results

In this section, we present the numerical method for approximating the solutions of (1) and state the main result of this paper.

2.1. Semidiscrete Galerkin FEM. We first only consider the case of discretization in space. 2

Let $\mathcal{T}_h$ be a quasi-uniform triangulation of the domain Ω into d-dimensional simplexes, denoted by π_h, with a mesh size h $(0 < h < h_0)$. A continuous piecewise linear finite element space X_h over the triangulation $\mathcal{T}_h$ is defined by

$$X_h = \{\chi_h \in H_0^1(\Omega) : \chi_h|_{\pi_h} \text{ is a linear function}, \forall \pi_h \in \mathcal{T}_h\}.$$

Over the finite element space X_h, we define the L^2 projection $P_h : L^2(\Omega) \to X_h$ by

$$(P_h\varphi, \chi_h) = (\varphi, \chi_h) \quad \forall \chi_h \in X_h$$

and define the discrete Laplacian $\Delta_h : X_h \to X_h$ by

$$(\Delta_h \varphi_h, \phi_h) = -(\nabla \varphi_h, \nabla \phi_h) \quad \forall \varphi_h, \phi_h \in X_h.$$

It is well-known that the L^2 projection satisfies the following standard error estimates ([20])

$$\|P_h \varphi\| \le C\|\varphi\| \qquad \forall \varphi \in L^2(\Omega) \tag{4}$$

$$\|P_h \varphi - \varphi\| \le Ch^2 \|\varphi\|_{H^2(\Omega)} \qquad \forall \varphi \in H^2(\Omega) \cap H_0^1(\Omega) \tag{5}$$

and the discrete Laplacian operator Δ_h satisfies the resolvent estimate (cf. [20, Chapter 6] and [1, Example 3.7.5 and Theorem 3.7.11])

$$\|(z - \Delta_h)^{-1}\| \le C|z|^{-1} \tag{6}$$

for any $z \in \Sigma_\theta := \{z \in \mathbb{C}\backslash\{0\} : |\arg z| \le \theta\}$ with $\theta \in (\pi/2, \pi)$. Then there exists a constant C, which depends only on θ and α, such that

$$\|(z^\alpha - \Delta_h)^{-1}\| \le C|z|^{-\alpha} \quad \forall z \in \Sigma_\theta. \tag{7}$$

With the above notations, the spatially semidiscrete Galerkin FEM for problem (1) is to find $u_h(t) \in v_h + X_h$ such that

$$(\partial_t u_h, \chi_h) + (\nabla \partial_t^{1-\alpha} u_h, \nabla \chi_h) = (f, \chi_h) \quad \forall \chi_h \in X_h \tag{8}$$

with the initial condition $u_h(0) := v_h = P_h v \in X_h$. Through the discrete Laplacian Δ_h, we can rewrite the semidiscrete Galerkin FEM (8) in the following equivalent form:

$$\partial_t u_h(t) - \Delta_h \partial_t^{1-\alpha} u_h(t) = f_h(t) \quad \forall t > 0 \tag{9}$$

with $u_h(0) = v_h$ and $f_h(t) = P_h f(t)$. It was shown in [6, setting $q_h = q$ in Lemma 3.2] that the semidiscrete scheme (9) has second-order convergence in space. In this paper, we focus on the error estimates for the time discretization of (9).

2.2. The Crank-Nicolson scheme. We now turn to time discretization of (9). Because the Caputo fractional derivative satisfies

$$\partial_t^{1-\alpha} u_h(x,t) = \partial_t^{1-\alpha}(u_h(x,t) - u_h(x,0)),$$

the equation (9) can be equivalently written as

$$\partial_t(u_h(t) - v_h) - \Delta_h \partial_t^{1-\alpha}(u_h(t) - v_h) = f_h(t). \tag{10}$$

Let $\{t_n = n\tau\}_{n=0}^N$ denote a uniform partition of the time interval $[0,T]$, with a step size $\tau = T/N$, and $u^n = u(x, t_n)$. We approximate the fractional derivative $\partial_t^{1-\alpha}(u_h(t_n) - v_h)$ by the backward Euler CQ (cf. [14, 18] and [9, (2.4)]):

$$\bar\partial_\tau^{1-\alpha}(u_h^n - v_h) := \frac{1}{\tau^{1-\alpha}} \sum_{j=1}^{n} b_{n-j}(u_h^j - v_h), \quad n = 1, 2, \ldots, N, \tag{11}$$

where the coefficients b_j, $j = 0, 1, 2, \ldots$, are determined by the power series expansion

$$(1 - \xi)^{1-\alpha} = \sum_{j=0}^{\infty} b_j \xi^j \quad \forall \xi \in \mathbb{C} \text{ such that } |\xi| < 1.$$

For any sequence $\{g^n\}_{n=0}^\infty \in \ell^2(L^2(\Omega))$, we denote the generating function of the sequence by

$$\widetilde{g}(\xi) = \sum_{n=0}^{\infty} g^n \xi^n \quad \text{for } \xi \in \mathbb{D}, \tag{12}$$

that is an $L^2(\Omega)$-valued analytic function in the unit disk $\mathbb{D}$ and the limit

$$\widetilde{g}(e^{i\theta}) = \lim_{r\to 1_-} \widetilde{g}(re^{i\theta})$$

exists in $L^2(0,2\pi;L^2(\Omega))$. Then, we have

$$\begin{aligned}\sum_{n=0}^{\infty}(\bar\partial_\tau^{1-\alpha}g^n)\xi^n &= \sum_{n=0}^{\infty}\frac{1}{\tau^{1-\alpha}}\sum_{j=0}^{n}b_{n-j}g^j\xi^n \\ &= (\tfrac{1-\xi}{\tau})^{1-\alpha}\sum_{j=0}^{\infty}g^j\xi^j = (\tfrac{1-\xi}{\tau})^{1-\alpha}\widetilde{g}(\xi).\end{aligned} \tag{13}$$

Besides, we define the standard backward Euler difference operator

$$\bar\partial_\tau u_h^n := \frac{u_h^n - u_h^{n-1}}{\tau}, \quad n = 1,2,\ldots,N. \tag{14}$$

If the solution u_h is smooth in time, then the backward Euler CQ has truncation error $O(\tau)$, namely, $\bar\partial_\tau^{1-\alpha}(u_h^n - v_h) - \partial_t^{1-\alpha}u_h(t_n) = O(\tau)$ at the nodes t_n, $n = 1,2,\ldots,N$. Recently, it was observed in [2, 4, 9] that such an approximation is $O(\tau^2)$ at the shifted point $t = t_n - \frac{1-\alpha}{2}\tau$, i.e.,

$$\bar\partial_\tau^{1-\alpha}(u_h^n - v_h) = \partial_t^{1-\alpha}u_h(t_n - \tfrac{1-\alpha}{2}\tau) + O(\tau^2),$$

which implies

$$\begin{aligned}&\partial_t^{1-\alpha}u_h(t_n - \tfrac{\tau}{2}) \\ &= (1-\tfrac{\alpha}{2})\partial_t^{1-\alpha}u_h(t_n - \tfrac{1-\alpha}{2}\tau) + \tfrac{\alpha}{2}\partial_t^{1-\alpha}u_h(t_{n-1} - \tfrac{1-\alpha}{2}\tau) + O(\tau^2) \\ &= (1-\tfrac{\alpha}{2})\bar\partial_\tau^{1-\alpha}(u_h^n - v_h) + \tfrac{\alpha}{2}\bar\partial_\tau^{1-\alpha}(u_h^{n-1} - v_h) + O(\tau^2).\end{aligned}$$

The above result inspires us to propose the following time-stepping scheme: find $U_h^n \in X_h$ such that

$$\begin{aligned}&\bar\partial_\tau(U_h^n - v_h) - (1-\tfrac{\alpha}{2})\Delta_h\bar\partial_\tau^{1-\alpha}(U_h^n - v_h) - \tfrac{\alpha}{2}\Delta_h\bar\partial_\tau^{1-\alpha}(U_h^{n-1} - v_h) \\ &= \tfrac{1}{2}(f_h^n + f_h^{n-1})\end{aligned} \tag{15}$$

for $n = 1,2,\ldots,N$, with $U_h^0 = v_h$ and $f_h^n = f_h(t_n)$.

For the above Crank-Nicolson scheme, we prove the following convergence result.

Theorem 2.1. *For $f \in W^{2,1}(0,T;L^2(\Omega))$, the solutions of* (9) *and* (15) *satisfy the estimate*

$$\|u_h(t_n) - U_h^n\| \le C\tau^2\left(t_n^{-1}\|f(0)\| + \|f'(0)\| + \int_0^{t_n}\|f''(s)\|\mathrm{d}s\right), \tag{16}$$

where the constant C is independent of h, τ, n, v, and f (but may depend on T).

Remark 2.1. *In* (1)*, the boundary condition $\partial_t^{1-\alpha}u(x,t) = 0$ is equivalent to $u(x,t) - v(x) = 0$ on $\partial\Omega \times \mathbb{R}_+$, where $v(x)$ is the initial value.*

Remark 2.2. *For initial data $v \in L^2(\Omega)$ and source $f \in L^1(0,T;L^2(\Omega))$, the problem* (1) *admits a mild solution $u \in C([0,T];L^2(\Omega))$* [5, Appendix A]. *When the Caputo derivative of order $\alpha \in (0,1)$ is used in* (1) *with $f = 0$, $u_h(t_n) = U_h^n = v_h$ for $n = 0,1,\ldots,N$, and thus the error estimate above does not depend on the regularity of the initial data. This is different from the case $\alpha \in (1,2)$ considered in* [3, 14] *and also different from the case of using Riemann-Liouville derivative in* (1).

3. Proof of Theorem 2.1

In this section, we establish the error estimates of the Crank-Nicolson scheme (15). The theoretical analysis is based on an integral representation of the solutions, which will be first presented in the following subsection.

3.1. Solution representations. In this subsection, we derive the integral representations of the semidiscrete solution $\omega_h(t) := u_h(t) - v_h$ and the fully discrete solution $W_h^n := U_h^n - v_h$, respectively.

Clearly, it follows from (10) that the function ω_h satisfies

$$\partial_t \omega_h(t) - \Delta_h \partial_t^{1-\alpha} \omega_h(t) = f_h(t)$$

with $\omega_h(0) = 0$. By applying the Laplace transform, we have

$$z\widehat{\omega}_h(z) - z^{1-\alpha}\Delta_h \widehat{\omega}_h(z) = \widehat{f}_h(z),$$

where z is a complex number and $\widehat{\omega}_h(z)$ denotes the Laplace transform of $\omega_h(t)$, i.e., $\widehat{\omega}_h(z) = \int_0^{+\infty} e^{-zt}\omega_h(t)\mathrm{d}t$. Taking the inverse Laplace transform, the function $\omega_h(t)$ can be represented as

$$\begin{aligned} \omega_h(t) &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}} e^{zt} z^{\alpha-1}(z^\alpha - \Delta_h)^{-1} \widehat{f}_h(z) \mathrm{d}z \\ &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}} e^{zt} K(z) \widehat{f}_h(z) \mathrm{d}z, \end{aligned} \tag{17}$$

with the kernel function defined by $K(z) = z^{\alpha-1}(z^\alpha - \Delta_h)^{-1}$. Here, $\Gamma_{\theta,\kappa}$ denotes a contour on the complex plane defined by

$$\Gamma_{\theta,\kappa} = \{z \in \mathbb{C} : |z| = \kappa, |\arg z| \le \theta\} \cup \{z \in \mathbb{C} : z = \rho e^{\pm \mathrm{i}\theta}, \rho \ge \kappa\}. \tag{18}$$

The angle θ above can be any angle such that $\pi/2 < \theta < \min(\pi, \pi/\alpha)$ so that, for all z to the right of $\Gamma_{\theta,\kappa}$ in the complex plane, $z^\alpha \in \Sigma_{\alpha\theta} := \{z \in \mathbb{C}\backslash\{0\} : |\arg z^\alpha| \le \alpha\theta\}$ with $\alpha\theta < \pi$.

In the following, by means of the discrete analogues of Laplace transform and generating function, we derive an integral representation of the fully discrete solution W_h^n over a truncated contour $\Gamma_{\theta,\kappa}^\tau$ defined by

$$\Gamma_{\theta,\kappa}^\tau := \{z \in \Gamma_{\theta,\kappa} : |\mathrm{Im}(z)| \le \pi/\tau\}. \tag{19}$$

Proposition 3.1. *Let $K(z) := z^{\alpha-1}(z^\alpha - \Delta_h)^{-1}$ and $G_h^n := f_h^n - f_h^0$. Then, the fully discrete solution W_h^n can be represented by*

$$\begin{aligned} W_h^n = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} \Big(& \mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{-1} K(\beta_\tau(e^{-z\tau})) f_h^0 \\ & + K(\beta_\tau(e^{-z\tau}))\gamma(e^{-z\tau})\widetilde{G}_h(e^{-z\tau})\tau \Big) \mathrm{d}z \end{aligned} \tag{20}$$

with integration over the truncated contour $\Gamma_{\theta,\kappa}^\tau$ defined in (19) *(oriented with increasing imaginary parts), and the parameters κ and θ satisfying the conditions of Lemma 3.1 below. In the representation* (20)*, the functions $\beta_\tau(\xi)$, $\mu(\xi)$, and $\gamma(\xi)$ are given by*

(21)

$$\beta_\tau(\xi) = \frac{1-\xi}{\tau(1-\frac{\alpha}{2}+\frac{\alpha}{2}\xi)^{1/\alpha}}, \quad \mu(\xi) = \frac{\xi}{(1-\frac{\alpha}{2}+\frac{\alpha}{2}\xi)^{2/\alpha}}, \quad \gamma(\xi) = \frac{\frac{1}{2}+\frac{1}{2}\xi}{(1-\frac{\alpha}{2}+\frac{\alpha}{2}\xi)^{1/\alpha}},$$

respectively.

Proof. The scheme (15) shows that the fully discrete solution W_h^n satisfies

$$\bar\partial_\tau W_h^n - (1-\tfrac{\alpha}{2})\Delta_h \bar\partial_\tau^{1-\alpha} W_h^n - \tfrac{\alpha}{2}\bar\partial_\tau^{1-\alpha} W_h^n = \tfrac12 (f_h^n + f_h^{n-1}) \tag{22}$$

for $n = 1, 2, \dots, N$, with $W_h^0 = 0$. Without loss of generality, we can assume $f_h^n = f_h^0$ (i.e., $G_h^n = 0$) for $n > N = T/\tau$. Otherwise, we can define $f_h^n := f_h^0$ for $n > N$. It is seen from (22) that such definition does not affect the value of W_h^n for $n = 1, 2, \dots, N$. Then, by multiplying (22) by ξ^n on both sides and summing up the results for $n = 1, 2, \dots,$ we get

$$\begin{aligned}&\sum_{n=1}^\infty \xi^n \bar\partial_\tau W_h^n - \sum_{n=1}^\infty \big[(1-\tfrac{\alpha}{2})\Delta_h \bar\partial_\tau^{1-\alpha} W_h^n + \tfrac{\alpha}{2}\Delta_h \bar\partial_\tau^{1-\alpha} W_h^{n-1}\big]\xi^n \\ &= \sum_{n=1}^\infty \tfrac12 (f_h^n + f_h^{n-1})\xi^n.\end{aligned} \tag{23}$$

Noting that $W_h^0 = 0$, by the discrete convolution rule, we have

$$\begin{aligned}&\sum_{n=1}^\infty \xi^n \bar\partial_\tau W_h^n = \tau^{-1}(1-\xi)\widetilde W_h(\xi),\\ &\sum_{n=1}^\infty \big[(1-\tfrac{\alpha}{2})\Delta_h \bar\partial_\tau^{1-\alpha} W_h^n + \tfrac{\alpha}{2}\Delta_h \bar\partial_\tau^{1-\alpha} W_h^{n-1}\big]\xi^n\\ &= (1-\tfrac{\alpha}{2}+\tfrac{\alpha}{2}\xi)\tau^{-(1-\alpha)}(1-\xi)^{1-\alpha}\Delta_h \widetilde W_h(\xi),\end{aligned}$$

and

$$\begin{aligned}\sum_{n=1}^\infty \tfrac12 (f_h^n + f_h^{n-1})\xi^n &= \sum_{n=1}^\infty \tfrac12 (G_h^n + G_h^{n-1})\xi^n + \sum_{n=1}^n f_h^0 \xi^n\\ &= (\tfrac12 + \tfrac12\xi)\widetilde G_h(\xi) + f_h^0 \xi (1-\xi)^{-1}.\end{aligned}$$

Since $|\xi| < 1$, $\beta_\tau(\xi)^\alpha \in \Sigma_{\theta'}$ for some $\theta' \in (\pi/2, \pi)$ (cf. [8, proof of Theorem 6.1]). By the resolvent estimate (7), substituting the above results into (23) leads to

$$\begin{aligned}\widetilde W_h(\xi) &= (\beta_\tau(\xi)^\alpha - \Delta_h)^{-1}\bigg(\frac{\tau^{1-\alpha}\xi}{(1-\xi)^{2-\alpha}(1-\frac{\alpha}{2}+\frac{\alpha}{2}\xi)} f_h^0 \\ &\qquad + \frac{\tau^{1-\alpha}(\frac12+\frac12\xi)}{(1-\xi)^{1-\alpha}(1-\frac{\alpha}{2}+\frac{\alpha}{2}\xi)}\widetilde G_h(\xi)\bigg)\\ &= \frac{1}{\tau}\mu(\xi)\beta_\tau(\xi)^{-1}K(\beta_\tau(\xi)) f_h^0 + K(\beta_\tau(\xi))\gamma(\xi)\widetilde G_h(\xi).\end{aligned} \tag{24}$$

We note that $\widetilde W_h(\xi)$ is analytic with respect to ξ in a neighborhood of the origin. Hence, using Cauchy's integral formula, we derive

$$W_h^n = \frac{1}{2\pi \mathrm{i}}\int_{|\xi|=\rho} \xi^{-n-1}\widetilde W_h(\xi)\mathrm{d}\xi = \frac{\tau}{2\pi\mathrm{i}}\int_{\Gamma_\rho^\tau} e^{zt_n}\widetilde W_h(e^{-z\tau})\mathrm{d}z$$

for $\rho \in (0,1)$, where the second equality is obtained by the change of variables $\xi = e^{-z\tau}$, and Γ_ρ^τ denotes the segment of a vertical line defined by

$$\Gamma_\rho^\tau := \{z = -\ln(\rho)/\tau + \mathrm{i}y \;:\; y \in \mathbb{R} \text{ and } |y| \le \pi/\tau\}. \tag{25}$$

Lemma 3.1 below shows that the operator $(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}$ is analytic with respect to z in the region $\Sigma \in \mathbb{C}$ enclosed by the curves Γ_ρ^τ, $\Gamma_{\theta,\kappa}^\tau$, and the two lines $\mathbb{R} \pm \mathrm{i}\pi/\tau$ (oriented from left to right). Consequently, it is easily seen that $e^{zt_n}\widetilde W_h(e^{-z\tau})$ is analytic with respect to $z \in \Sigma$. Furthermore, it is straightforward to prove that the values of $e^{zt_n}\widetilde{W}_h(e^{-z\tau})$ on the two lines $\mathbb{R}\pm \mathrm{i}\pi/\tau$ coincide. Thus, by using Cauchy's theorem, we get

$$\begin{aligned} W_h^n &= \frac{\tau}{2\pi \mathrm{i}}\int_{\Gamma_\rho^\tau} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\mathrm{d}z \\ &= \frac{\tau}{2\pi \mathrm{i}}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\mathrm{d}z + \frac{\tau}{2\pi \mathrm{i}}\int_{\mathbb{R}+\frac{\mathrm{i}\pi}{\tau}} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\mathrm{d}z \\ &\quad - \frac{\tau}{2\pi \mathrm{i}}\int_{\mathbb{R}-\frac{\mathrm{i}\pi}{\tau}} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\mathrm{d}z \\ &= \frac{\tau}{2\pi \mathrm{i}}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}\widetilde{W}_h(e^{-z\tau})\mathrm{d}z, \end{aligned} \tag{26}$$

with which, the desired result (20) follows immediately. □

In (17) and (20), the integral representations of the semidiscrete solution and the fully discrete numerical solution have been derived, respectively. Before we prove the error estimates of the numerical scheme (15), we introduce several useful lemmas in the following.

Lemma 3.1. *(*[9, Lemma 3.3]*) For $\alpha \in (0,1)$, let $\phi \in (\alpha\pi/2, \pi)$ be fixed. Then there exists a constant $\kappa_0 > 0$ (independent of τ) such that for $\kappa \in (0, \kappa_0]$ and $\theta \in (\pi/2, \pi/2+\kappa_0]$, we have*

$$\beta_\tau(e^{-z\tau})^\alpha \in \Sigma_\phi \quad \forall z \in \Gamma_{\theta,\kappa}^\tau \cup \overline{\Sigma}_{\pi/2}/\{0\}. \tag{27}$$

Moreover, the operator $(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}$ is analytic with respect to z in the region enclosed by the curves Γ_ρ^τ, $\Gamma_{\theta,\kappa}^\tau$ and $\mathbb{R}\pm i\pi/\tau$ and satisfies

$$\|(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\| \le C|\beta_\tau(e^{-z\tau})|^{-\alpha} \quad \forall z \in \Gamma_{\theta,\kappa}^\tau, \tag{28}$$

where the constant C is independent of τ (but may depend on ϕ).

Lemma 3.2. *Let $\alpha \in (0,1)$ be given, and $\beta_\tau(\xi)$, $\mu(\xi)$, $\gamma(\xi)$ be defined as in* (21)*. Then there exists a constant $\kappa_1 > 0$ (independent of τ) such that for $\kappa \in (0,\kappa_1]$ and $\theta \in (\pi/2, \pi/2+\kappa_1]$, we have for any $z \in \Gamma_{\theta,\kappa}^\tau$,*

$$|\mu(e^{-z\tau})| \le C \tag{29}$$

$$|\gamma(e^{-z\tau})| \le C \tag{30}$$

$$|\mu(e^{-z\tau}) - 1| \le C\tau^2|z|^2 \tag{31}$$

$$|\gamma(e^{-z\tau}) - 1| \le C\tau^2|z|^2 \tag{32}$$

and

$$C_0|z| \le |\beta_\tau(e^{-z\tau})| \le C_1|z| \tag{33}$$

$$|\beta_\tau(e^{-z\tau}) - z| \le C\tau^2|z|^3 \tag{34}$$

$$|\beta_\tau(e^{-z\tau})^\alpha - z^\alpha| \le C\tau^2|z|^{2+\alpha}, \tag{35}$$

where the constants C_0, C_1 and C are independent of τ, θ and κ (but may depend on κ_1).

Proof. The proof of the estimates (33)-(35) can be found in [9, Lemma 3.4]. By using Taylor expansion, the estimates (29)-(32) can be easily obtained. □

3.2. Error analysis of the numerical scheme. In the homogeneous case $f \equiv 0$, we have $u_h(t_n) = U_h^n = v_h$ for $n = 0, 1, \ldots, N$, and thus Theorem 2.1 follows immediately. Therefore, it remains to consider the inhomogeneous case $f \neq 0$ with zero initial $v = 0$. Using Taylor expansion, we have

$$f_h(t) = f_h(0) + t f_h'(0) + t * f_h'', \tag{36}$$

where $*$ denotes the convolution. By linearity, it suffices to consider the three cases $f_h = f_h(0)$, $tf_h'(0)$ and $t * f_h''$, separately.

We begin with error estimates for the case $f_h(t) = f_h(0) =: f_h^0$.

Lemma 3.3. *Let $v = 0$, and $u_h(t)$ and U_h^n denote the solutions of* (9) *and* (15) *with the source term $f_h(t) = f_h^0$ and $f_h^n = f_h^0$, respectively. For $f_h^0 \in L^2(\Omega)$, we have*

$$\|u_h(t_n) - U_h^n\| \le C\tau^2 t_n^{-1} \|f_h^0\|, \tag{37}$$

where the constant C is independent of τ.

Proof. Let κ_0 and κ_1 be the constants defined in Lemma 3.1 and Lemma 3.2, respectively. By choosing $\kappa = \min(\kappa_0, \kappa_1)$ and $\theta = \frac{\pi}{2} + \kappa$, (17) and (20) yield

$$u_h(t_n) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}} e^{zt_n} z^{\alpha-2} (z^\alpha - \Delta_h)^{-1} f_h^0 \mathrm{d}z \quad (\text{here we use } \widehat{f_h^0}(z) = \tfrac{1}{z} f_h^0) \tag{38}$$

$$U_h^n = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} \mu(e^{-z\tau}) \beta_\tau(e^{-z\tau})^{\alpha-2} (\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1} f_h^0 \mathrm{d}z. \tag{39}$$

Therefore, we have

$$\begin{aligned} &u_h(t_n) - U_h^n \\ &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} [z^{\alpha-2}(z^\alpha - \Delta_h)^{-1} - \mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{\alpha-2}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}] f_h^0 \mathrm{d}z \\ &\quad + \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}/\Gamma_{\theta,\kappa}^\tau} e^{zt_n} z^{\alpha-2}(z^\alpha - \Delta_h)^{-1} f_h^0 \mathrm{d}z \\ &=: \mathcal{I}_1 + \mathcal{I}_2. \end{aligned}$$

Clearly, the analysis of $\mathcal{I}_1$ is based on the error bound of the kernel $z^{\alpha-2}(z^\alpha - \Delta_h)^{-1}$ to $\mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{\alpha-2}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}$ along the contour $\Gamma_{\theta,\kappa}^\tau$. Hence, we first prove the following result:

$$\|z^{\alpha-2}(z^\alpha - \Delta_h)^{-1} - \mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{\alpha-2}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\| \le C\tau^2 \tag{40}$$

for any $z \in \Gamma_{\theta,\kappa}^\tau$. By the triangle inequality, we have

$$\begin{aligned} &\|z^{\alpha-2}(z^\alpha - \Delta_h)^{-1} - \mu(e^{-z\tau})\beta_\tau(e^{-z\tau})^{\alpha-2}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\| \\ &\le |\mu(e^{-z\tau}) - 1| \|z^{\alpha-2}(z^\alpha - \Delta_h)^{-1}\| \\ &\quad + |\mu(e^{-z\tau})| \|z^{\alpha-2}(z^\alpha - \Delta_h)^{-1} - \beta_\tau(e^{-z\tau})^{\alpha-2}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\| \\ &=: A_1 + A_2. \end{aligned}$$

With Lemma 3.2 and the resolvent estimate (7), it shows

$$A_1 \le C\tau^2 |z|^2 |z|^{\alpha-2} |z|^{-\alpha} \le C\tau^2.$$

Since

$$
\begin{aligned}
&|\beta_\tau(e^{-z\tau})^{\alpha-2} - z^{\alpha-2}| \\
&\leq |z^2\beta_\tau(e^{-z\tau})^{\alpha} - \beta_\tau(e^{-z\tau})^2 z^{\alpha}||\beta_\tau(e^{-z\tau})|^{-2}|z|^{-2} \\
&\leq \big(|z^2(\beta_\tau(e^{-z\tau})^{\alpha} - z^{\alpha})| + |(z^2 - \beta_\tau(e^{-z\tau})^2)z^{\alpha}|\big)|\beta_\tau(e^{-z\tau})|^{-2}|z|^{-2} \\
&\leq C\tau^2|z|^{\alpha}
\end{aligned}
$$

and $\|(z^\alpha - \Delta_h)^{-1} - (\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\| \leq C\tau^2|z|^{2-\alpha}$ (cf. [9, the estimate of (3.20)]), we have

$$
\begin{aligned}
A_2 &\leq |\beta_\tau(e^{-z\tau})^{\alpha-2} - z^{\alpha-2}|\|(z^\alpha - \Delta_h)^{-1}\| \\
&\quad + |\beta_\tau(e^{-z\tau})^{\alpha-2}|\|(z^\alpha - \Delta_h)^{-1} - (\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\| \\
&\leq C\tau^2.
\end{aligned}
$$

Combining the estimates of A_1 and A_2 yields (40).

With (40) and choosing $\kappa = 1/t_n$, we derive

$$
\begin{aligned}
\|\mathcal{I}_1\| &\leq C\tau^2\|f_h^0\|\left(\int_\kappa^{\frac{\pi}{\tau\sin\theta}} e^{rt_n\cos\theta}\mathrm{d}r + \int_{-\theta}^{\theta} e^{\kappa t_n|\cos\varphi|}\kappa\mathrm{d}\varphi\right) \\
&\leq C\tau^2\|f_h^0\|(t_n^{-1} + \kappa) \\
&\leq C\tau^2 t_n^{-1}\|f_h^0\|.
\end{aligned}
$$

Furthermore, since $\|z^{\alpha-2}(z^\alpha - \Delta_h)^{-1}\| \leq C|z|^{\alpha-2}|z|^{-\alpha} \leq C|z|^{-2}$, we get

$$
\begin{aligned}
\|\mathcal{I}_2\| &\leq C\|f_h^0\|\int_{\frac{\pi}{\tau\sin\theta}}^{\infty} e^{rt_n\cos\theta}r^{-2}\mathrm{d}r \\
&\leq C\tau^2\|f_h^0\|\int_0^\infty e^{rt_n\cos\theta}\mathrm{d}r \quad (\text{here we use } r \geq \tfrac{\pi}{\tau\sin\theta}) \\
&\leq C\tau^2 t_n^{-1}\|f_h^0\|.
\end{aligned}
$$

This completes the proof of Lemma 3.3. □

Next, we consider the error estimates for the source term of the form $f_h(t) = tf_h'(0)$.

Lemma 3.4. *Let $v = 0$, and $u_h(t)$ and U_h^n denote the solutions of* (9) *and* (15) *with the source term $f_h = tf_h'(0)$ and $f_h^n = t_n f_h'(0)$, respectively. For $f_h'(0) \in L^2(\Omega)$, we have*

(41) $$\|u_h(t_n) - U_h^n\| \leq C\tau^2\|f_h'(0)\|,$$

where the constant C is independent of τ.

Proof. Again, let κ_0 and κ_1 be the constants defined in Lemma 3.1 and Lemma 3.2, respectively. By choosing $\kappa = \min(\kappa_0, \kappa_1)$ and $\theta = \frac{\pi}{2} + \kappa$, it follows from (17) and (20) that

(42)
$$u_h(t_n) = \frac{1}{2\pi\mathrm{i}}\int_{\Gamma_{\theta,\kappa}} e^{zt_n}z^{\alpha-3}(z^\alpha - \Delta_h)^{-1}f_h'(0)\mathrm{d}z \quad (\text{here use } \widehat{f}_h(z) = \tfrac{1}{z^2}f_h'(0))$$

(43)
$$U_h^n = \frac{1}{2\pi\mathrm{i}}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}\frac{\tau^2 e^{-z\tau}}{(1 - e^{-z\tau})^2}\beta_\tau(e^{-z\tau})^{\alpha-1}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\gamma(e^{-z\tau})f_h'(0)\mathrm{d}z.$$

Then, we have

$$
\begin{aligned}
&u_h(t_n) - U_h^n \\
&= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} \Big(z^{\alpha-3}(z^\alpha - \Delta_h)^{-1} \\
&\qquad - \frac{\tau^2 e^{-z\tau}}{(1-e^{-z\tau})^2} \beta_\tau(e^{-z\tau})^{\alpha-1}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\gamma(e^{-z\tau})\Big) f_h'(0)\mathrm{d}z \\
&\quad + \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}/\Gamma_{\theta,\kappa}^\tau} e^{zt_n} z^{\alpha-3}(z^\alpha - \Delta_h)^{-1} f_h'(0)\mathrm{d}z \\
&=: \mathcal{J}_1 + \mathcal{J}_2.
\end{aligned}
$$

Similarly as the proof of Lemma 3.3, we shall show below the error estimates of the kernels:

$$
\begin{aligned}
&\left\| z^{\alpha-3}(z^\alpha - \Delta_h)^{-1} - \frac{\tau^2 e^{-z\tau}}{(1-e^{-z\tau})^2} \beta_\tau(e^{-z\tau})^{\alpha-1}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\gamma(e^{-z\tau}) \right\| \\
&\le c\tau^2 |z|^{-1} \qquad (44)
\end{aligned}
$$

for any $z \in \Gamma_{\theta,\kappa}^\tau$. By the triangle inequality, we have

$$
\begin{aligned}
&\left\| z^{\alpha-3}(z^\alpha - \Delta_h)^{-1} - \frac{\tau^2 e^{-z\tau}}{(1-e^{-z\tau})^2} \beta_\tau(e^{-z\tau})^{\alpha-1}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\gamma(e^{-z\tau}) \right\| \\
&\le |z^{\alpha-1} - \beta_\tau(e^{-z\tau})^{\alpha-1}||z|^{-2}\|(z^\alpha - \Delta_h)^{-1}\| \\
&\quad + |\beta_\tau(e^{-z\tau})|^{\alpha-1}|z|^{-2}\|(z^\alpha - \Delta_h)^{-1} - (\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\| \\
&\quad + |\beta_\tau(e^{-z\tau})|^{\alpha-1}|z|^{-2}\|(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\||1 - \gamma(e^{-z\tau})| \\
&\quad + |\beta_\tau(e^{-z\tau})|^{\alpha-1}\|(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\||\gamma(e^{-z\tau})|\left| z^{-2} - \frac{\tau^2 e^{-z\tau}}{(1-e^{-z\tau})^2}\right| \\
&=: D_1 + D_2 + D_3 + D_4.
\end{aligned}
$$

Now, we analyse D_i, $1 \le i \le 4$, respectively. Since

$$
\begin{aligned}
&|\beta_\tau(e^{-z\tau})^{\alpha-1} - z^{\alpha-1}| \\
&\le |z\beta_\tau(e^{-z\tau})^\alpha - \beta_\tau(e^{-z\tau})z^\alpha||\beta_\tau(e^{-z\tau})|^{-1}|z|^{-1} \\
&\le \big(|z||\beta_\tau(e^{-z\tau})^\alpha - z^\alpha| + |z - \beta_\tau(e^{-z\tau})||z|^\alpha\big)|\beta_\tau(e^{-z\tau})|^{-1}|z|^{-1} \\
&\le C\tau^2|z|^{\alpha+1},
\end{aligned}
$$

it turns out

$$D_1 \le C\tau^2|z|^{\alpha+1}|z|^{-2}|z|^\alpha \le C\tau^2|z|^{-1}.$$

By the resolvent estimate (7), Lemmas 3.1 and 3.2, we further have

$$
\begin{aligned}
D_2 &\le C|z|^{\alpha-1}|z|^{-2}\tau^2|z|^{2-\alpha} \le C\tau^2|z|^{-1}, \\
D_3 &\le C|z|^{\alpha-1}|z|^{-2}|z|^{-\alpha}\tau^2|z|^2 \le C\tau^2|z|^{-1}.
\end{aligned}
$$

To obtain the estimate of D_4, we note that $|(1-e^{-z\tau})^2 e^{z\tau}\tau^{-2} - z^2| \le C\tau^2|z|^4$ (cf. [9, Lemma 3.11]) and $|(1-e^{-z\tau})^2 e^{z\tau}\tau^{-2}z^2| \ge c|z|^4$ (straightforward to prove by applying the same method as used in (C.1) in [5]), which imply

$$\left| z^{-2} - \frac{\tau^2 e^{-z\tau}}{(1-e^{-z\tau})^2}\right| \le C\tau^2.$$

Using Lemma 3.2, we have

$$D_4 \le C|\beta_\tau(e^{-z\tau})|^{\alpha-1}|\beta_\tau(e^{-z\tau})|^{-\alpha}\tau^2 \le C\tau^2|z|^{-1}.$$

Combining the estimates of D_i, $1 \le i \le 4$, results in (44).

With the estimate (44) and choosing $\kappa = 1/t_n$, we have

$$\|\mathcal{J}_1\| \le C\tau^2\|f_h'(0)\|\left(\int_\kappa^{\frac{\pi}{\tau\sin\theta}} e^{rt_n\cos\theta}r^{-1}\mathrm{d}r + \int_{-\theta}^{\theta} e^{\kappa t_n|\cos\varphi|}\mathrm{d}\varphi\right) \le C\tau^2\|f_h'(0)\|.$$

By the resolvent estimate (7), it follows that

$$\begin{aligned}\|\mathcal{J}_2\| &\le C\|f_h'(0)\|\int_{\frac{\pi}{\tau\sin\theta}}^{\infty} e^{rt_n\cos\theta}r^{-3}\mathrm{d}r\\ &\le C\tau^2\|f_h'(0)\|\int_{\frac{\pi}{\tau\sin\theta}}^{\infty} e^{rt_n\cos\theta}r^{-1}\mathrm{d}r \quad (\text{here we use } r \ge \tfrac{\pi}{\tau\sin\theta})\\ &\le C\tau^2\|f_h'(0)\|.\end{aligned}$$

The proof of Lemma 3.4 is complete. □

Finally, we present the error estimates for the source term of the form $f_h(t) = t * f_h''$.

Lemma 3.5. *Let $v = 0$, and $u_h(t)$ and U_h^n denote the solutions of* (9) *and* (15) *with the source term $f_h(t) = t * f_h''$ and $f_h^n = t * f_h''$, respectively. For $f_h \in W^{2,1}(0,T;L^2(\Omega))$, we have*

$$\|u_h(t_n) - U_h^n\| \le C\tau^2\int_0^{t_n}\|f_h''(s)\|\mathrm{d}s, \tag{45}$$

where the constant C is independent of τ.

Proof. In this part, we still choose $\kappa = \min(\kappa_0, \kappa_1)$ and $\theta = \frac{\pi}{2} + \kappa$. Similarly as the analysis in [9], we introduce an operator $\mathcal{E}(t)$ defined by

$$\mathcal{E}(t) = \frac{1}{2\pi\mathrm{i}}\int_{\Gamma_{\theta,\kappa}} e^{zt}z^{\alpha-1}(z^\alpha - \Delta_h)^{-1}\mathrm{d}z. \tag{46}$$

With such an operator and using the Laplace transform of the convolution quadrature, it follows from (17) that the semidiscrete Galerkin solution $u_h(t_n)$ can be represented by

$$u_h(t_n) = (\mathcal{E} * f_h)(t_n) = (\mathcal{E} * (t * f_h''))(t_n) = ((\mathcal{E} * t) * f_h'')(t_n). \tag{47}$$

By using the Laplace transform of the convolution quadrature again, it is seen from (46) that

$$(\mathcal{E} * t)(t) = \frac{1}{2\pi\mathrm{i}}\int_{\Gamma_{\theta,\kappa}} e^{zt}z^{\alpha-3}(z^\alpha - \Delta_h)^{-1}\mathrm{d}z. \tag{48}$$

To establish the error estimate (45) for the source term $t * f_h''$, we shall below derive a similar representation of the fully discrete solution U_h^n as $u_h(t_n)$ in (47). Since $\beta_\tau(\xi)^{\alpha-1}(\beta_\tau(\xi)^\alpha - \Delta_h)^{-1}\gamma(\xi)$ is analytic with respect to ξ in a neighborhoood of the origin, it can be represented by a generating function, i.e.,

$$\beta_\tau(\xi)^{\alpha-1}(\beta_\tau(\xi)^\alpha - \Delta_h)^{-1}\gamma(\xi) = \sum_{n=0}^{\infty}\mathcal{E}_\tau^n\xi^n. \tag{49}$$

Applying the similar method as used in Proposition 3.1 (by Cauchy's integral formula and Cauchy's theorem), it is easy to see that

$$\mathcal{E}_\tau^n = \frac{\tau}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} \beta_\tau(e^{-z\tau})^{\alpha-1}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\gamma(e^{-z\tau})\mathrm{d}z.$$

Since $v = 0$ and by (24), we obtain

$$\begin{aligned}\widetilde{U}_h(\xi) &= (\beta_\tau(\xi)^\alpha - \Delta_h)^{-1} \frac{\tau^{1-\alpha}(\frac{1}{2}+\frac{1}{2}\xi)}{(1-\xi)^{1-\alpha}(1-\frac{\alpha}{2}+\frac{\alpha}{2}\xi)} \widetilde{f}_h(\xi) \\ &= \beta_\tau(\xi)^{\alpha-1}(\beta_\tau(\xi)^\alpha - \Delta_h)^{-1}\gamma(\xi)\widetilde{f}_h(\xi) \\ &= \Big(\sum_{n=0}^\infty \mathcal{E}_\tau^n \xi^n\Big)\Big(\sum_{n=0}^\infty f_h(t_n)\xi^n\Big) \\ &= \sum_{n=0}^\infty U_h^n \xi^n, \end{aligned} \tag{50}$$

where we have used (49) and the definition of generating function, i.e., $\widetilde{f}_h(\xi) = \sum_{n=0}^\infty f_h(t_n)\xi^n$. The above last equality further implies

$$U_h^n = \sum_{j=0}^n \mathcal{E}_\tau^{n-j} f_h(t_j).$$

Let $\mathcal{E}_\tau(t) = \sum_{n=0}^\infty \mathcal{E}_\tau^n \delta_{t_n-\epsilon}(t)$ with $\delta_{t_n-\epsilon}$ denoting the Dirac delta function concentrated at $t_n - \epsilon$ and ϵ an arbitrary small constant. Then, we have

$$U_h^n = \lim_{\epsilon\to 0}(\mathcal{E}_\tau * f_h)(t_n) = \lim_{\epsilon\to 0}(\mathcal{E}_\tau * (t * f_h''))(t_n) = \lim_{\epsilon\to 0}((\mathcal{E}_\tau * t) * f_h'')(t_n). \tag{51}$$

From (47) and (51), it suffices to analyse the error estimates of $(\mathcal{E} - \mathcal{E}_\tau) * t$. By using the definition of $\mathcal{E}_\tau(t)$, it clearly shows $\lim_{\epsilon\to 0}(\mathcal{E}_\tau * t)(t_n) = \sum_{j=0}^n \mathcal{E}_\tau^{n-j} t_j$. Hence, with (49), we get the following generating function

$$\begin{aligned}\sum_{n=0}^\infty \lim_{\epsilon\to 0}(\mathcal{E}_\tau * t)(t_n)\xi^n &= \sum_{n=0}^\infty \sum_{j=0}^n \mathcal{E}_\tau^{n-j} t_j \xi^n = \Big(\sum_{n=0}^\infty \mathcal{E}_\tau^n \xi^n\Big)\Big(\sum_{n=0}^\infty t_n \xi^n\Big) \\ &= \beta_\tau(\xi)^{\alpha-1}(\beta_\tau(\xi)^\alpha - \Delta_h)^{-1}\gamma(\xi)\frac{\tau\xi}{(1-\xi)^2}.\end{aligned}$$

Again, using the similar method given in Proposition 3.1 (by Cauchy's integral formula and Cauchy's theorem), it shows that

$$\begin{aligned}&\lim_{\epsilon\to 0}(\mathcal{E}_\tau * t)(t_n) \\ &= \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} \frac{\tau^2 e^{-z\tau}}{(1-e^{-z\tau})^2} \beta_\tau(e^{-z\tau})^{\alpha-1}(\beta_\tau(e^{-z\tau})^\alpha - \Delta_h)^{-1}\gamma(e^{-z\tau})\mathrm{d}z.\end{aligned} \tag{52}$$

Applying the same technique as used in Lemma 3.4, we obtain

$$\Big\| \lim_{\epsilon\to 0}((\mathcal{E} - \mathcal{E}_\tau) * t)(t_n) \Big\| \le C\tau^2. \tag{53}$$

Next, we prove that the same result still holds for any $t \in (t_{n-1}, t_n)$, i.e.,

$$\Big\| \lim_{\epsilon\to 0}((\mathcal{E} - \mathcal{E}_\tau) * t)(t) \Big\| \le C\tau^2 \quad \forall t \in (t_{n-1}, t_n). \tag{54}$$

To this end, we take the Taylor expansion of $\mathcal{E}(t)$ at $t = t_n$:

$$(\mathcal{E} * t)(t) = (\mathcal{E} * t)(t_n) + (t - t_n)(\mathcal{E} * 1)(t_n) + \int_{t_n}^t (t-s)\mathcal{E}(s)\mathrm{d}s.$$

Such expansion also holds for $(\mathcal{E}_\tau * t)(t)$. Thus, to derive the estimate (54), we first prove the following result

$$\left\| \lim_{\epsilon\to 0}((\mathcal{E}-\mathcal{E}_\tau)*1)(t_n)\right\| \le C\tau. \tag{55}$$

By using the definition of the operator $\mathcal{E}(t)$ in (46), we arrive at

$$(\mathcal{E}*1)(t) = \frac{1}{2\pi\mathrm{i}}\int_{\Gamma_{\theta,\kappa}} e^{zt} z^{\alpha-2}(z^\alpha-\Delta_h)^{-1}\mathrm{d}z.$$

Recalling the definition of $\mathcal{E}_\tau(t)=\sum_{n=0}^\infty \mathcal{E}_\tau^n \delta_{t_n-\epsilon}(t)$, we have

$$\begin{aligned}\sum_{n=0}^\infty \lim_{\epsilon\to 0}(\mathcal{E}_\tau*1)(t_n)\xi^n &= \sum_{n=0}^\infty\sum_{j=0}^n \mathcal{E}_\tau^{n-j}\xi^n = \Big(\sum_{n=0}^\infty \mathcal{E}_\tau^n\xi^n\Big)\Big(\sum_{n=0}^\infty \xi^n\Big)\\ &= \beta_\tau(\xi)^{\alpha-1}(\beta_\tau(\xi)^\alpha-\Delta_h)^{-1}\gamma(\xi)\frac{1}{1-\xi},\end{aligned}$$

which implies

$$\lim_{\epsilon\to 0}(\mathcal{E}_\tau*1)(t_n) = \frac{1}{2\pi\mathrm{i}}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}\frac{\tau}{1-e^{-z\tau}}\beta_\tau(e^{-z\tau})^{\alpha-1}(\beta_\tau(e^{-z\tau})^\alpha-\Delta_h)^{-1}\gamma(e^{-z\tau})\mathrm{d}z.$$

To prove (55), we shall show below the error bound of the kernels $z^{\alpha-2}(z^\alpha-\Delta_h)^{-1}$ to $\frac{\tau}{1-e^{-z\tau}}\beta_\tau(e^{-z\tau})^{\alpha-1}(\beta_\tau(e^{-z\tau})^\alpha-\Delta_h)^{-1}\gamma(e^{-z\tau})$. The proof is analogous to that of (44). By the triangle inequality, we have

$$\begin{aligned}&\left\| z^{\alpha-2}(z^\alpha-\Delta_h)^{-1} - \frac{\tau}{1-e^{-z\tau}}\beta_\tau(e^{-z\tau})^{\alpha-1}(\beta_\tau(e^{-z\tau})^\alpha-\Delta_h)^{-1}\gamma(e^{-z\tau})\right\|\\ &\le |z|^{-1}\|(z^\alpha-\Delta_h)^{-1}\||z^{\alpha-1}-\beta_\tau(e^{-z\tau})^{\alpha-1}|\\ &\quad + |z|^{-1}|\beta_\tau(e^{-z\tau})|^{\alpha-1}\|(z^\alpha-\Delta_h)^{-1}-(\beta_\tau(e^{-z\tau})^\alpha-\Delta_h)^{-1}\|\\ &\quad + |z|^{-1}|\beta_\tau(e^{-z\tau})|^{\alpha-1}\|(\beta_\tau(e^{-z\tau})^\alpha-\Delta_h)^{-1}\||1-\gamma(e^{-z\tau})|\\ &\quad + |\beta_\tau(e^{-z\tau})|^{\alpha-1}\|(\beta_\tau(e^{-z\tau})^\alpha-\Delta_h)^{-1}\||\gamma(e^{-z\tau})|\left|z^{-1}-\frac{\tau}{1-e^{-z\tau}}\right|\\ &\le C\tau^2 + C\tau|z|^{-1},\end{aligned}$$

where we have used $|z^{-1}-\tau(1-e^{-z\tau})^{-1}|\le C\tau$. With such estimate, we derive

$$\begin{aligned}&\left\| \lim_{\epsilon\to 0}((\mathcal{E}-\mathcal{E}_\tau)*1)(t_n)\right\|\\ &\le C\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}(\tau^2+\tau|z|^{-1})\mathrm{d}z + C\int_{\Gamma_{\theta,\kappa}\setminus\Gamma_{\theta,\kappa}^\tau} e^{zt_n}|z|^{-2}\mathrm{d}z\\ &\le C\left(\int_\kappa^{\frac{\pi}{\tau\sin\theta}} e^{rt_n\cos\theta}(\tau^2+\tau r^{-1})\mathrm{d}r + \int_{-\theta}^{\theta} e^{\kappa t_n|\cos\varphi|}(\tau^2\kappa+\tau)\mathrm{d}\varphi\right)\\ &\quad + C\int_{\frac{\pi}{\tau\sin\theta}}^\infty e^{rt_n\cos\theta}r^{-2}\mathrm{d}r\\ &\le C\left(\int_\kappa^{\frac{\pi}{\tau\sin\theta}} e^{rt_n\cos\theta}\tau r^{-1}\mathrm{d}r + C(\tau^2\kappa+\tau)\right) \quad (\text{here we use } \tau\le \tfrac{\pi}{r\sin\theta})\\ &\quad + C\tau\int_{\frac{\pi}{\tau\sin\theta}}^\infty e^{rt_n\cos\theta}r^{-1}\mathrm{d}r \quad (\text{here we use } r\ge \tfrac{\pi}{\tau\sin\theta})\\ &\le C\tau,\end{aligned}$$

which is (55). Finally, since $\|z^{\alpha-1}(z^\alpha - \Delta_h)^{-1}\| \le C|z|^{-1}$, it implies

$$\|\mathcal{E}(t)\| \le C\int_\kappa^\infty e^{rt\cos\theta} r^{-1}\mathrm{d}r + C\int_{-\theta}^{\theta} e^{\kappa t_n|\cos\varphi}\mathrm{d}\varphi \le C,$$

and therefore,

$$\left\|\int_{t_n}^t (t-s)\mathcal{E}(s)\mathrm{d}s\right\| \le C\int_t^{t_n}(s-t)\mathrm{d}s \le C\tau^2.$$

With $\|\mathcal{E}_\tau^n\| \le C\tau$ (straightforward to prove), we further get

$$\left\|\int_{t_n}^t (t-s)\mathcal{E}_\tau(s)\mathrm{d}s\right\| \le \tau\|\mathcal{E}_\tau^n\| \le C\tau^2.$$

Combining the above results yields the estimate (54). Together with (47) and (51), the proof of Lemma 3.5 is complete. □

By using the estimate (4) and Lemmas 3.3-3.5, Theorem 2.1 follows immediately.

4. Numerical examples

In this section, we present a numerical example to illustrate the performance of the fully discrete Crank-Nicolson scheme (15) for solving (1) in the one-dimensional spacial domain $\Omega = (0,1)$ up to time $T = 1$, with two pairs of given v and f, i.e.,

$$\text{(a) } v = \sin(\pi x),\ \ f = 2e^t\sin(\pi x)$$
$$\text{(b) } v = x(1-x),\ \ f = 5(1+t^{1.5})x(1-x),$$

where the functions f in both (a) and (b) satisfy the regularity assumptions of Theorem 2.1.

TABLE 1. The L^2 error $\|u_h(t_n) - U_h^n\|$ for Example (a).

$\alpha\backslash\tau_k$	2^{-3}	2^{-4}	2^{-5}	2^{-6}	order
$\alpha = 0.25$	1.626e-04	3.959e-05	9.736e-06	2.389e-06	2.030
$\alpha = 0.50$	9.948e-05	2.364e-05	5.732e-06	1.396e-06	2.052
$\alpha = 0.75$	8.069e-05	1.949e-05	4.760e-06	1.163e-06	2.039

TABLE 2. The L^2 error $\|u_h(t_n) - U_h^n\|$ for Example (b).

$\alpha\backslash\tau_k$	2^{-3}	2^{-4}	2^{-5}	2^{-6}	order
$\alpha = 0.25$	1.057e-04	2.694e-05	6.822e-06	1.705e-06	1.985
$\alpha = 0.50$	8.240e-05	2.099e-05	5.306e-06	1.325e-06	1.986
$\alpha = 0.75$	6.159e-05	1.574e-05	3.972e-06	9.895e-07	1.986

The problem (1) is discretized by using continuous piecewise linear finite element in space. Since the exact solution is unknown, we solve (1) by using a much finer mesh size $h = 2^{-8}$ and a smaller time step $\tau = 2^{-9}$ to compute the reference solution $u_h(t)$. Here, we only focus on the time discretization of (1) and measure the L^2 error $\|u_h(t_n) - U_h^n\|$ for different $\alpha \in (0,1)$. From Theorem 2.1, we might expect $\|u_h(t_n) - U_h^n\|$ to be $O(\tau^2)$. Thus, we choose the time step $\tau_k = 2^{-k}$, $k = 3,4,5,6$, and take a sufficiently small mesh size $h = 2^{-8}$ to avoid the effect of spatial discretization error. The numerical results for Examples (a) and (b) at the time $t = 1$ are given in Tables 1 and 2, which illustrate second-order accuracy in time.

Acknowledgments.

The research of M. Gunzburger and J. Wang was supported in part by the USA National Science Foundation grant DMS-1315259 and by the USA Air Force Office of Scientific Research grant FA9550-15-1-0001.

References

[1] W. Arendt, C. J. Batty, M. Hieber, and F. Neubrander. *Vector-valued Laplace Transforms and Cauchy Problems, Second Edition*. Birkhäuser, second edition, 2011.

[2] B. Baeumer, M. Kovács, and H. Sankaranarayanan. Higher order Grünwald approximations of fractional derivatives and fractional powers of operators. *Trans. Amer. Math. Soc.*, 367:813–834, 2015.

[3] E. Cuesta, C. Lubich, and C. Palencia. Convolution quadrature time discretization of fractional diffusion-wave equations. *Math. Comp.*, 75(254):673–696, 2006.

[4] Y. Dimitrov. Numerical approximations for fractional differential equations. *J. Fract. Calc. Appl.*, 5(suppl. 3S):Paper no. 22, 45, 2014.

[5] M. Gunzburger, B. Li, and J. Wang. Convergence of finite element solutions of stochastic partial integro-differential equations driven by the space-time white noise. *arXiv:1711.01998v1*, 2017.

[6] M. Gunzburger and J. Wang. Error analysis of fully discrete finite element approximations to an optimal control problem governed by a time-fractional PDE. *submitted*, 2017.

[7] B. Jin, R. Lazarov, and Z. Zhou. Two fully discrete schemes for fractional diffusion and diffusion-wave equations with nonsmooth data. *SIAM J. Sci. Comput.*, 38(1):A146–A170, 2016.

[8] B. Jin, B. Li, and Z. Zhou. Discrete Maximal Regularity of Time-Stepping Schemes for Fractional Evolution Equations. *Numer. Math.*, 2017, DOI: 10.1007/s00211-017-0904-8.

[9] B. Jin, B. Li, and Z. Zhou. An Analysis of the Crank-Nicolson Method for Subdiffusion. *IMA J. Numer. Anal.*, 2017, DOI: 10.1093/imanum/drx019.

[10] B. Jin, B. Li, and Z. Zhou. Correction of high-order BDF convolution quadrature for fractional evolution equations. *SIAM J. Sci. Comput.*, 2017, in press.

[11] A. A. Kilbas, H. M. Srivastava, and J. J. Trujillo. *Theory and Application of Fractional Differential Equations*. Elsecier Science B.V., Amsterdam, 2006.

[12] C. Lubich. Discretized fractional calculus. *SIAM J. Math. Anal.*, 17(3):704–719, 1986.

[13] C. Lubich. Convolution quadrature and discretized operational calculus. I. *Numer. Math.*, 52(2):129–145, 1988.

[14] C. Lubich, I. H. Sloan, and V. Thomée. Nonsmooth data error estimates for approximations of an evolution equation with a positive-type memory term. *Math. Comp.*, 65(213):1–17, 1996.

[15] W. McLean. Regularity of solutions to a time-fractional diffusion equation. *ANZIAM J.*, 52:123–138, 2010.

[16] W. McLean and K. Mustapha. A second-order accurate numerical method for a fractional wave equation. *Numer. Math.*, 105(3):481–510, 2007.

[17] W. McLean and K. Mustapha. Time-stepping error bounds for fractional diffusion problems with non-smooth initial data. *J. Comput. Phys.*, 293:201–217, 2015.

[18] J. M. Sanz-Serna. A numerical method for a partial integro-differential equation. *SIAM J. Numer. Anal.*, 25(2):319–327, 1988.

[19] Z.-Z. Sun and X. Wu. A fully discrete scheme for a diffusion wave system. *Appl. Numer. Math.*, 56(2):193–209, 2006.

[20] V. Thomée. *Galerkin Finite Element Methods for Parabolic Problems*. Springer-Verlag, Berlin, 2nd edition, 2006.

[21] L. Vázquez, M. P. Velasco, J. L. Vázquez-Poletti, I. M. Llorente, D. Usero, and S. Jiménez. Modeling and simulation of the atmospheric dust dynamic: fractional calculus and cloud computing. *Int. J. Numer. Anal. & Model.*, 15:74–85, 2018.

Department of Scientific Computing, Florida State University, Tallahassee, FL 32306, USA
E-mail: mgunzburger@fsu.edu, jwang13@fsu.edu

Department of Mathematics and Statistics, Mississippi State University, Starkville, MS 39762, USA
E-mail: jwang@math.msstate.edu