

ERROR ANALYSIS OF A FINITE ELEMENT METHOD FOR THE SPACE-FRACTIONAL PARABOLIC EQUATION*

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Abstract. We consider an initial boundary value problem for a one-dimensional fractional-order parabolic equation with a space fractional derivative of Riemann–Liouville type and order $\alpha \in (1, 2)$. We study a spatial semidiscrete scheme using the standard Galerkin finite element method with piecewise linear finite elements, as well as fully discrete schemes based on the backward Euler method and the Crank–Nicolson method. Error estimates in the $L^2(D)$ - and $H^{\alpha/2}(D)$ -norm are derived for the semidiscrete scheme and in the $L^2(D)$ -norm for the fully discrete schemes. These estimates cover both smooth and nonsmooth initial data and are expressed directly in terms of the smoothness of the initial data. Extensive numerical results are presented to illustrate the theoretical results.

Key words. finite element method, space fractional parabolic equation, semidiscrete scheme, fully discrete scheme, error estimate

AMS subject classifications. 65M60, 65N30, 65N15

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1. Introduction. We consider the following initial boundary value problem for a space fractional-order parabolic differential equation for $u(x, t)$:

$$(1.1) \quad \begin{aligned} u_t - {}_0^R D_x^\alpha u &= f, & x \in D = (0, 1), & 0 < t \leq T, \\ u(0, t) = u(1, t) &= 0, & 0 < t \leq T, \\ u(x, 0) &= v, & x \in D, \end{aligned}$$

where $\alpha \in (1, 2)$ is the order of the fractional derivative, the source term f belongs to $L^2(0, T; L^2(D))$, and the initial data v belongs to $L^2(D)$ or its suitable subspace. The notation ${}_0^R D_x^\alpha u$ refers to the Riemann–Liouville derivative of order α , defined in (2.1) below, and $T > 0$ is fixed. In case of $\alpha = 2$, the fractional derivative ${}_0^R D_x^\alpha u$ coincides with the usual second-order derivative u'' [13], and then model (1.1) recovers the classical diffusion equation.

The classical diffusion equation is often used to describe transport process. The use of a Laplace operator in the equation rests on a Brownian motion assumption on the random motion of individual particles. However, over the last few decades, a number of studies [1, 9, 15] have shown that anomalous diffusion, in which the mean square variance grows faster (superdiffusion) or slower (subdiffusion) than that in a Gaussian process, offers a superior fit to experimental data observed in some processes, e.g., viscoelastic materials, soil contamination, and underground water flow.

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In particular, at a microscopic level, the particle motion might be dependent, and can frequently take very large steps, following some heavy-tailed probability distribution. The long-range correlation and large jumps can cause the underlying stochastic process to deviate significantly from Brownian motion for the classical diffusion process. Instead, a Lévy process is considered to be more appropriate. The macroscopic counterpart is the space fractional diffusion equation (SpFDE) (1.1), and we refer to [1] for the derivation and relevant physical explanations. Numerous experimental studies have shown that it can provide an accurate description of the superdiffusion process.

Because of the extraordinary modeling capability of (1.1), its accurate numerical solution has become an important task. A number of numerical methods, prominently the finite difference method, have been developed for the time-dependent superdiffusion process in the literature. The finite difference scheme is usually based on a shifted Grünwald formula for the Riemann–Liouville fractional derivative in space. In [17, 18], the stability, consistency, and convergence were shown for the finite difference scheme with the Crank–Nicolson scheme in time. In these works, the convergence rates are provided under the a priori assumption that the solution u to (1.1) is sufficiently smooth, which unfortunately is not justified in general; cf. Theorem 3.2.

In this work, we develop a finite element method for (1.1) and analyze the convergence rates for both space semidiscrete and fully discrete schemes. To the best of our knowledge, it represents the first theoretical work for the SpFDE (1.1) with nonsmooth data. It is based on the variational formulation of the space fractional boundary value problem, initiated in [2, 3] and recently revisited in [12]. We establish $L^2(D)$ - and $\tilde{H}^{\alpha/2}(D)$ -norm error estimates for the space semidiscrete scheme and $L^2(D)$ -norm estimates for fully discrete schemes, using analytic semigroup theory [10]. Specifically, we obtain the following results. First, in Theorem 3.1 we establish the existence and uniqueness of a weak solution $u \in L^2(0, T; \tilde{H}^{\alpha/2}(D))$ of (1.1) (see section 2 for the definitions of the space $\tilde{H}^\beta(D)$ and the operator A) and in Theorem 3.2 show an enhanced regularity $u \in C((0, T]; \tilde{H}_L^{\alpha-1+\beta}(D))$ with $\beta \in [1 - \alpha/2, 1/2)$ for $v \in L^2(D)$. Second, in Theorems 4.5 and 4.3 we show that the semidiscrete finite element solution $u_h(t)$ with suitable discrete initial value $u_h(0)$ satisfies the a priori error bound

$$\begin{aligned} & \|u_h(t) - u(t)\|_{L^2(D)} + h^{\alpha/2-1+\beta} \|u_h(t) - u(t)\|_{\tilde{H}^{\alpha/2}(D)} \\ & \leq Ch^{\alpha-2+2\beta} t^{l-1} \|A^l v\|_{L^2(D)}, \quad l = 0, 1, \end{aligned}$$

with h being the mesh size and any $\beta \in [1 - \alpha/2, 1/2)$. Further we derived error estimates for the fully discrete solution U^n , with τ being the time step size and $t_n = n\tau$, for the backward Euler method and the Crank–Nicolson method. For the backward Euler method, in Theorems 5.2 and 5.3, we establish the error estimates

$$\|u(t_n) - U^n\|_{L^2(D)} \leq C(h^{\alpha-2+2\beta} + \tau)t_n^{l-1} \|A^l v\|_{L^2(D)}, \quad l = 0, 1,$$

and for the Crank–Nicolson method, in Theorems 5.5 and 5.7, we prove

$$\|u(t_n) - U^n\|_{L^2(D)} \leq C(h^{\alpha-2+2\beta} + \tau^2 t_n^{-1}) t_n^{l-1} \|A^l v\|_{L^2(D)}, \quad l = 0, 1.$$

These error estimates cover both smooth and nonsmooth initial data and the bounds are directly expressed in terms of the initial data v . This is in sharp contrast with existing studies which assume directly the regularity of the solution. The case of nonsmooth initial data is especially interesting in inverse problems and optimal control.

The rest of the paper is organized as follows. In section 2, we describe preliminaries on fractional derivatives and related continuous and discrete variational formulations. Then in section 3, we discuss the existence and uniqueness of a weak solution to (1.1) using a Galerkin procedure and show the regularity pickup by the semigroup theory. Further, the properties of the discrete semigroup $E_h(t)$ are discussed. The error analysis for the semidiscrete scheme is carried out in section 4, and that for fully discrete schemes based on the backward Euler method and the Crank–Nicolson method is provided in section 5. Numerical results for smooth and nonsmooth initial data are presented in section 6. Throughout, we use the notation c and C , with or without a subscript, to denote a generic constant, which may change at different occurrences, but it is always independent of the solution u , time t , mesh size h , and time step size τ .

2. Fractional derivative and variational formulation. In this part, we describe fundamentals of fractional calculus, the variational problem for the source problem with a Riemann–Liouville fractional derivative, and discuss the finite element discretization.

2.1. Fractional derivative. We first briefly recall the Riemann–Liouville fractional derivative. For any positive noninteger real number β with $n - 1 < \beta < n$, $n \in \mathbb{N}$, the left-sided Riemann–Liouville fractional derivative ${}^R_0D_x^\beta u$ of order β of a function $u \in C^n[0, 1]$ is defined by [13, p. 70]

$$(2.1) \quad {}^R_0D_x^\beta u = \frac{d^n}{dx^n} ({}_0I_x^{n-\beta} u).$$

Here ${}_0I_x^\gamma$ for $\gamma > 0$ is the left-sided Riemann–Liouville fractional integral operator of order γ defined by

$$({}_0I_x^\gamma f)(x) = \frac{1}{\Gamma(\gamma)} \int_0^x (x-t)^{\gamma-1} f(t) dt,$$

where $\Gamma(\cdot)$ is Euler’s Gamma function defined by $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$. The right-sided versions of fractional-order integral and derivative are defined analogously, i.e.,

$$({}_xI_1^\gamma f)(x) = \frac{1}{\Gamma(\gamma)} \int_x^1 (t-x)^{\gamma-1} f(t) dt \quad \text{and} \quad {}^R_xD_1^\beta u = (-1)^n \frac{d^n}{dx^n} ({}_xI_1^{n-\beta} u).$$

Now we introduce some function spaces. For any $\beta \geq 0$, we denote $H^\beta(D)$ to be the Sobolev space of order β on the unit interval $D = (0, 1)$ and $\tilde{H}^\beta(D)$ to be the set of functions in $H^\beta(D)$ whose extension by zero to \mathbb{R} is in $H^\beta(\mathbb{R})$. Analogously, we define $\tilde{H}_L^\beta(D)$ (respectively, $\tilde{H}_R^\beta(D)$) to be the set of functions u whose extension by zero \tilde{u} is in $H^\beta(-\infty, 1)$ (respectively, $H^\beta(0, \infty)$). Here for $u \in \tilde{H}_L^\beta(D)$, we set $\|u\|_{\tilde{H}_L^\beta(D)} := \|\tilde{u}\|_{H^\beta(-\infty, 1)}$ with an analogous definition for the norm in $\tilde{H}_R^\beta(D)$. The fractional derivative operator ${}^R_0D_x^\beta$ is well defined for functions in $C^n[0, 1]$ and can be extended continuously from $\tilde{H}_L^\alpha(D)$ to $L^2(D)$ [2, Lemma 2.6], [12, Theorem 2.2].

2.2. Variational formulation and its discretization. Now we recall the variational formulation for the source problem

$$-{}^R_0D_x^\alpha u = f$$

with $u(0) = u(1) = 0$, and $f \in L^2(D)$. The proper variational formulation is given by [12]: find $u \in V \equiv \tilde{H}^{\alpha/2}(D)$ such that

$$(2.2) \quad A(u, \psi) = (f, \psi) \quad \forall \psi \in V,$$

where the sesquilinear form $A(\cdot, \cdot)$ is given by

$$A(\varphi, \psi) = -({}_0^R D_x^{\alpha/2} \varphi, {}_x^R D_1^{\alpha/2} \psi).$$

It is known [2, Lemma 3.1], [12, Lemma 4.2] that the sesquilinear form $A(\cdot, \cdot)$ is coercive on the space V , i.e., there is a constant c_0 such that for all $\psi \in V$

$$(2.3) \quad \Re A(\psi, \psi) \geq c_0 \|\psi\|_{\tilde{H}^{\alpha/2}(D)}^2,$$

where \Re denotes taking the real part, and continuous on V , i.e., for all $\varphi, \psi \in V$

$$(2.4) \quad |A(\varphi, \psi)| \leq C_0 \|\varphi\|_{\tilde{H}^{\alpha/2}(D)} \|\psi\|_{\tilde{H}^{\alpha/2}(D)}.$$

Then by the Riesz representation theorem, there exists a unique bounded linear operator $\tilde{A} : \tilde{H}^{\alpha/2}(D) \rightarrow \tilde{H}^{\alpha/2}(D)$ such that

$$A(\varphi, \psi) = \langle \tilde{A}\varphi, \psi \rangle \quad \forall \varphi, \psi \in \tilde{H}^{\alpha/2}(D).$$

Define $D(A) = \{\psi \in \tilde{H}^{\alpha/2}(D) : \tilde{A}\psi \in L^2(D)\}$ and an operator $A : D(A) \rightarrow L^2(D)$ by

$$(2.5) \quad A(\varphi, \psi) = (A\varphi, \psi), \quad \varphi \in D(A), \psi \in \tilde{H}^{\alpha/2}(D).$$

Remark 2.1. The domain $D(A)$ has a complicated structure: it consists of functions of the form ${}_0 I_x^\alpha f - ({}_0 I_x^\alpha f)(1)x^{\alpha-1}$, where $f \in L^2(D)$ [12]. The term $x^{\alpha-1} \in \tilde{H}_L^{\alpha-1+\beta}(D)$, $\beta \in [1 - \alpha/2, 1/2)$, appears because it is in the kernel of the operator ${}_0^R D_x^\alpha$. Hence, $D(A) \subset \tilde{H}_L^{\alpha-1+\beta}(D) \cap \tilde{H}^{\alpha/2}(D)$ and it is dense in $L^2(D)$.

The next result shows that the linear operator A is sectorial, which means that (a) The resolvent set $\rho(A)$ contains the sector $\Sigma_\theta = \{z : \theta \leq |\arg z| \leq \pi\}$ for $\theta \in (0, \pi/2)$; (b) $\|(\lambda I - A)^{-1}\| \leq M/|\lambda|$ for $\lambda \in \Sigma_\theta$ and some constant M .

Then we have the following important lemma (cf. [10, p. 94, Theorem 3.6]), for which we sketch a proof for completeness.

LEMMA 2.1. *The linear operator A defined in (2.5) is sectorial on $L^2(D)$.*

Proof. For all $\varphi \in D(A)$, we obtain by (2.3) and (2.4)

$$|(A\varphi, \varphi)| \leq C_0 \|\varphi\|_{\tilde{H}^{\alpha/2}(D)}^2 \leq \frac{C_0}{c_0} \Re(A\varphi, \varphi).$$

Thus $\mathcal{N}(A)$, the numerical range of A , which is defined by

$$\mathcal{N}(A) = \{(A\varphi, \varphi) : \varphi \in D(A) \text{ and } \|\varphi\|_{L^2(D)} = 1\},$$

is contained in the sector $\Sigma_0 = \{z : 0 \leq |\arg(z)| \leq \delta_0\}$, with $\delta_0 = \arccos(c_0/C_0)$.

Now we choose $\delta_1 \in (\delta_0, \pi/2)$ and set $\Sigma_{\delta_1} = \{z : \delta_1 \leq |\arg(z)| \leq \pi\}$. Then by [8, p. 310, Proposition C.3.1], the resolvent set $\rho(A)$ contains Σ_{δ_1} and for all $\lambda \in \Sigma_{\delta_1}$

$$\|(\lambda I - A)^{-1}\| \leq \frac{1}{\text{dist}(\lambda, \overline{\mathcal{N}(A)})} \leq \frac{1}{\text{dist}(\lambda, \Sigma_0)} \leq \frac{1}{\sin(\delta_1 - \delta_0)} \frac{1}{|\lambda|}.$$

This completes the proof of this lemma. \square

The next corollary is an immediate consequence of Lemma 2.1.

COROLLARY 2.2. *The linear operator A is the infinitesimal generator of an analytic semigroup $E(t) = e^{-At}$ on $L^2(D)$.*

Proof. The proof follows directly from Lemma 2.1 and standard semigroup theory; cf. [10, Theorem 3.4, Proposition 3.9, and Theorem 3.19]. \square

2.3. Finite element discretization. We introduce a finite element approximation based on an equally spaced partition of the interval D . We let $h = 1/m$ be the mesh size with $m > 1$ being a positive integer and consider the nodes $x_j = jh$, $j = 0, \dots, m$. We then define V_h to be the set of continuous functions in V which are linear when restricted to the subintervals $[x_i, x_{i+1}]$, $i = 0, \dots, m-1$, i.e.,

$$V_h = \{\chi \in C_0(\overline{D}) : \chi \text{ is linear over } [x_i, x_{i+1}], i = 0, \dots, m\}.$$

We define the discrete operator $A_h : V_h \rightarrow V_h$ by

$$(A_h \varphi, \chi) = A(\varphi, \chi) \quad \forall \varphi, \chi \in V_h.$$

The lemma below is a direct corollary of (2.3) and (2.4).

LEMMA 2.3. *The discrete operator A_h satisfies*

$$\begin{aligned} \Re(A_h \psi, \psi) &\geq c_0 \|\psi\|_{\tilde{H}^{\alpha/2}(D)}^2, \quad \psi \in V_h, \\ |(A_h \varphi, \psi)| &\leq C_0 \|\varphi\|_{\tilde{H}^{\alpha/2}(D)} \|\psi\|_{\tilde{H}^{\alpha/2}(D)}, \quad \varphi, \psi \in V_h. \end{aligned}$$

Remark 2.2. By Lemma 2.3 and repeating the argument in the proof of Lemma 2.1, we can show that A_h is a sectorial operator on V_h with the same constant as A .

Next we recall the Ritz projection $R_h : \tilde{H}^{\alpha/2}(D) \rightarrow V_h$ and the $L^2(D)$ -projection $P_h : L^2(D) \rightarrow V_h$, respectively, defined by

$$(2.6) \quad \begin{aligned} A(R_h \psi, \chi) &= A(\psi, \chi) \quad \forall \psi \in \tilde{H}^{\alpha/2}(D), \chi \in V_h, \\ (P_h \varphi, \chi) &= (\varphi, \chi) \quad \forall \varphi \in L^2(D), \chi \in V_h. \end{aligned}$$

The operator R_h has the following approximation properties [12].

LEMMA 2.4. *For any $v \in D(A)$, the operator R_h satisfies for $\beta \in [1 - \alpha/2, 1/2]$*

$$\|v - R_h v\|_{L^2(D)} + h^{\alpha/2-1+\beta} \|v - R_h v\|_{\tilde{H}^{\alpha/2}(D)} \leq Ch^{\alpha-2+2\beta} \|Av\|_{L^2(D)}.$$

We shall also need the adjoint problem in the error analysis. Similar to (2.5), we define the adjoint operator A^* as

$$A(\varphi, \psi) = (\varphi, A^* \psi) \quad \forall \varphi \in \tilde{H}^{\alpha/2}(D), \psi \in D(A^*),$$

where the domain $D(A^*)$ of A^* satisfies $D(A^*) \subset \tilde{H}_R^{\alpha-1+\beta}(D) \cap \tilde{H}^{\alpha/2}(D)$ and it is dense in $L^2(D)$. Further, the discrete analogue A_h^* of A^* is defined by

$$A(\varphi, \psi) = (\varphi, A_h^* \psi) \quad \forall \varphi, \psi \in V_h.$$

Remark 2.3. In our discussions, we have restricted our attention to the case $A = -{}^R_0 D_x^\alpha$. The analysis can be extended to the more general case $A = -{}^R_0 D_x^\alpha + q$, with the potential $q \in L^\infty(D)$ and $q \geq 0$, since the coercivity and continuity of the respective bilinear form holds, and the related regularity theory remains valid.

3. Variational formulation of the fractional-order parabolic problem.

The variational formulation of problem (1.1) is to find $u(t) \in V$ such that

$$(3.1) \quad (u_t, \varphi) + A(u, \varphi) = (f, \varphi) \quad \forall \varphi \in V$$

and $u(0) = v$. We shall establish the well-posedness of the variational formulation (3.1) using a Galerkin procedure and an enhanced regularity estimate via analytic semigroup theory. Further, the properties of the discrete semigroup are discussed.

3.1. Existence and uniqueness of the weak solution. First we state the existence and uniqueness of a weak solution, following a Galerkin procedure [4]. To this end, we choose an orthogonal basis $\{\omega_k(x) = \sqrt{2} \sin k\pi x\}$ in both $L^2(D)$ and $H_0^1(D)$ and orthonormal in $L^2(D)$. In particular, by the construction, the $L^2(D)$ -orthogonal projection operator P into $\text{span}\{\omega_k\}$ is stable in both $L^2(D)$ and $H_0^1(D)$, and by interpolation, it is also stable in $\tilde{H}^\beta(D)$ for any $\beta \in [0, 1]$. Now we fix a positive integer m and look for a solution $u_m(t)$ of the form

$$u_m(t) := \sum_{k=1}^m c_k(t)\omega_k$$

such that for $k = 1, 2, \dots, m$

$$(3.2) \quad c_k(0) = (v, \omega_k), \quad (u'_m, \omega_k) + A(u_m, \omega_k) = (f, \omega_k), \quad 0 \leq t \leq T.$$

The existence and uniqueness of u_m follow directly from the standard theory for ordinary differential equation systems. With the finite-dimensional approximation u_m at hand, one can deduce the following existence and uniqueness result. The proof is rather standard, and it is given in Appendix A for completeness.

THEOREM 3.1. *Let $f \in L^2(0, T; L^2(D))$ and $v \in L^2(D)$. Then there exists a unique weak solution $u \in L^2(0, T; \tilde{H}^{\alpha/2}(D))$ of (3.1).*

Now we study the regularity of the solution u using semigroup theory [10]. By Corollary 2.2 and the classical semigroup theory, the solution u to the initial boundary value problem (1.1) with $f \equiv 0$ can be represented as

$$u(t) = E(t)v,$$

where $E(t) = e^{-tA}$ is the semigroup generated by the sectorial operator A ; cf. Corollary 2.2. Then we have an improved regularity by [16, p. 104, Corollary 1.5].

THEOREM 3.2. *For every $v \in L^2(D)$, the initial boundary value problem (3.1) with $f \equiv 0$ has a unique solution $u(x, t) \in C([0, T]; L^2(D)) \cap C((0, T]; D(A))$.*

Further, we have the following $L^2(D)$ estimate.

LEMMA 3.3. *For $0 \leq \gamma \leq 1$, there holds*

$$\|A^\gamma E(t)\psi\|_{L^2(D)} \leq Ct^{-\gamma}\|\psi\|_{L^2(D)}.$$

Proof. The cases $\gamma = 0$ and $\gamma = 1$ have been proved in [19, p. 91, Theorem 6.4(iii)]. With the contour $\Gamma = \{z : z = \rho e^{\pm i\delta_1}, \rho \geq 0\}$ and the resolvent $R(z; A) = (zI - A)^{-1}$, the case of $\gamma \in (0, 1)$ follows by

$$\begin{aligned} \|A^\gamma E(t)\psi\|_{L^2(D)} &= \left\| \frac{1}{2\pi i} \int_\Gamma z^\gamma e^{-zt} R(z; A)\psi dz \right\|_{L^2(D)} \\ &\leq C\|\psi\|_{L^2(D)} \int_0^\infty \rho^{\gamma-1} e^{-\rho t} d\rho \leq Ct^{-\gamma}\|\psi\|_{L^2(D)}. \quad \square \end{aligned}$$

3.2. Properties of the semigroup $E_h(t)$. Let $E_h(t) = e^{-A_h t}$ be the semigroup generated by the operator A_h . Then it satisfies a discrete analogue of Lemma 3.3.

LEMMA 3.4. *There exists a constant $C > 0$ such that for $\chi \in V_h$*

$$\|A_h^\gamma E_h(t)\chi\|_{L^2(D)} \leq Ct^{-\gamma}\|\chi\|_{L^2(D)}.$$

Proof. The proof follows directly from Remark 2.2 and Lemma 3.3. \square

Last we recall the Dunford–Taylor spectral representation of a rational function $r(A_h)$ of A_h , when $r(z)$ is bounded in a sector in the right half plane [19, Lemma 9.1].

LEMMA 3.5. *Let $r(z)$ be a rational function that is bounded for $|\arg z| \leq \delta_1$, $|z| \geq \epsilon > 0$, and for $|z| \geq R$. Then if $\epsilon > 0$ is so small that $\{z : |z| \leq \epsilon\} \subset \rho(A_h)$, we have*

$$r(A_h) = r(\infty)I + \frac{1}{2\pi i} \int_{\Gamma_\epsilon \cup \Gamma_\epsilon^R \cup \Gamma^R} r(z)R(z; A_h)dz,$$

where $R(z; A_h) = (zI - A_h)^{-1}$ is the resolvent operator, $\Gamma_\epsilon^R = \{z : |\arg z| = \delta_1, \epsilon \leq |z| \leq R\}$, $\Gamma_\epsilon = \{z : |z| = \epsilon, |\arg z| \leq \delta_1\}$, and $\Gamma^R = \{z : |z| = R, \delta_1 \leq |\arg z| \leq \pi\}$, and with the closed path of integration oriented in the negative sense.

Remark 3.1. The representation in Lemma 3.5 holds true for any function $f(z)$ which is analytic in a neighborhood of $\{z : |\arg z| \leq \delta_1, |z| \geq \epsilon\}$, including at $z = \infty$.

4. Error estimates for semidiscrete Galerkin FEM. In this section, we derive $L^2(D)$ - and $\tilde{H}^{\alpha/2}(D)$ -norm error estimates for the semidiscrete Galerkin FEM: find $u_h(t) \in V_h$ such that

$$(4.1) \quad (u_{h,t}, \varphi) + A(u_h, \varphi) = (f, \varphi) \quad \forall \varphi \in V_h, \quad T \geq t > 0. \quad u_h(0) = v_h,$$

where $v_h \in V_h$ is an approximation to the initial data v . We shall discuss the case of smooth and nonsmooth initial data, i.e., $v \in D(A)$ and $v \in L^2(D)$, separately.

4.1. Error estimate for nonsmooth initial data. First we consider nonsmooth initial data, i.e., $v \in L^2(D)$. We follow the approach due to Fujita and Suzuki [6]. We begin with an important lemma. Here we shall use the constant δ_1 and the contour $\Gamma = \{z : z = \rho e^{\pm i\delta_1}, \rho \geq 0\}$ defined in the proof of Lemma 2.1.

LEMMA 4.1. *There exists a constant $C > 0$ such that for any $\varphi \in \tilde{H}^{\alpha/2}(D)$ and $z \in \Gamma$*

$$|z| \|\varphi\|_{L^2(D)}^2 + \|\varphi\|_{\tilde{H}^{\alpha/2}(D)}^2 \leq C |z| \|\varphi\|_{L^2(D)}^2 - A(\varphi, \varphi).$$

Proof. We use the notation δ_0 and δ_1 from the proof of Lemma 2.1. Then we choose δ' such that $\delta' \in (\delta_0, \delta_1)$ and let $c' = C_0 \cos \delta'$; cf. Figure 1(a). By setting $\gamma = c_0 - c' > 0$, we have

$$\Re A(\varphi, \varphi) - \gamma \|\varphi\|_{\tilde{H}^{\alpha/2}(D)}^2 \geq c' \|\varphi\|_{\tilde{H}^{\alpha/2}(D)}^2 \geq \cos \delta' |A(\varphi, \varphi)|.$$

By dividing both sides by $\|\varphi\|_{L^2(D)}^2$, this yields

$$|A(\varphi, \varphi)| / \|\varphi\|_{L^2(D)}^2 \in \Sigma_\varphi = \{z : |\arg(z - \gamma \|\varphi\|_{\tilde{H}^{\alpha/2}(D)}^2 / \|\varphi\|_{L^2(D)}^2)| \leq \delta'\}.$$

Note that for $z \in \Gamma$, there holds (cf. Figure 1(a))

$$\text{dist}(z, \Sigma_\varphi) \geq |z| \sin(\delta_1 - \delta') + \gamma \|\varphi\|_{\tilde{H}^{\alpha/2}(D)}^2 / \|\varphi\|_{L^2(D)}^2 \sin \delta'.$$

Consequently, for $z \in \Gamma$ we get

$$(4.2) \quad \begin{aligned} |z| \|\varphi\|_{L^2(D)}^2 - A(\varphi, \varphi) &\geq \|\varphi\|_{L^2(D)}^2 \text{dist}(z, \Sigma_\varphi) \\ &\geq |z| \|\varphi\|_{L^2(D)}^2 \sin(\delta_1 - \delta') + \gamma \|\varphi\|_{\tilde{H}^{\alpha/2}(D)}^2 \sin \delta' \\ &\geq \frac{1}{C} (|z| \|\varphi\|_{L^2(D)}^2 + \|\varphi\|_{\tilde{H}^{\alpha/2}(D)}^2), \end{aligned}$$

and this completes the proof. \square

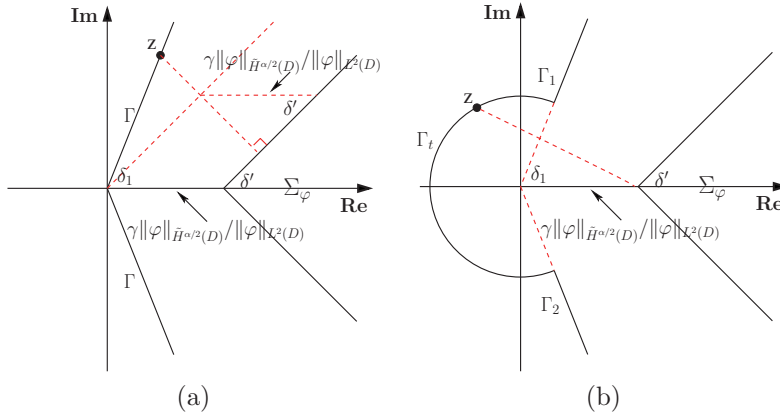


FIG. 1. The sectors Σ_{δ_1} and Σ_φ for (a) nonsmooth and (b) smooth initial data.

The next result gives estimates on $R(z; A)v$ and its discrete analogue.

LEMMA 4.2. *Let $v \in L^2(D)$, $z \in \Gamma$, $w = R(z; A)v$, and $w_h = R(z; A_h)P_h v$. Then for $\beta \in [1 - \alpha/2, 1/2)$, there holds*

$$(4.3) \quad \|w_h - w\|_{L^2(D)} + h^{\alpha/2-1+\beta} \|w_h - w\|_{\tilde{H}^{\alpha/2}(D)} \leq Ch^{\alpha-2+2\beta} \|v\|_{L^2(D)}.$$

Proof. By the definition, w and w_h satisfy, respectively,

$$\begin{aligned} z(w, \varphi) - A(w, \varphi) &= (v, \varphi) \quad \forall \varphi \in V, \\ z(w_h, \varphi) - A(w_h, \varphi) &= (v, \varphi) \quad \forall \varphi \in V_h. \end{aligned}$$

Subtracting these two identities gives an orthogonality relation for $e = w - w_h$:

$$(4.4) \quad z(e, \varphi) - A(e, \varphi) = 0 \quad \forall \varphi \in V_h.$$

This and Lemma 4.1 imply that for any $\chi \in V_h$

$$\begin{aligned} |z||e|_{L^2(D)}^2 + \|e\|_{\tilde{H}^{\alpha/2}(D)}^2 &\leq C|z||e|_{L^2(D)}^2 - A(e, e) \\ &= C|z|(e, w - \chi) - A(e, w - \chi). \end{aligned}$$

By taking $\chi = \pi_h w$, the finite element interpolant of w , and the Cauchy–Schwarz inequality, we obtain

$$(4.5) \quad \begin{aligned} |z||e|_{L^2(D)}^2 + \|e\|_{\tilde{H}^{\alpha/2}(D)}^2 &\leq C(|z|h^{\alpha/2}\|e\|_{L^2(D)}\|w\|_{\tilde{H}^{\alpha/2}(D)} \\ &\quad + h^{\alpha/2-1+\beta}\|e\|_{\tilde{H}^{\alpha/2}(D)}\|w\|_{H^{\alpha-1+\beta}(D)}). \end{aligned}$$

Appealing again to Lemma 4.1 with the choice $\varphi = w$, we arrive at

$$|z||w|_{L^2(D)}^2 + \|w\|_{\tilde{H}^{\alpha/2}(D)}^2 \leq C|((zI - A)w, w)| \leq C\|v\|_{L^2(D)}\|w\|_{L^2(D)}.$$

Consequently

$$(4.6) \quad \|w\|_{L^2(D)} \leq C|z|^{-1}\|v\|_{L^2(D)} \quad \text{and} \quad \|w\|_{\tilde{H}^{\alpha/2}(D)} \leq C|z|^{-1/2}\|v\|_{L^2(D)}.$$

It remains to bound $\|w\|_{H^{\alpha-1+\beta}(D)}$. To this end, we deduce from (4.6) that

$$\begin{aligned}\|w\|_{H^{\alpha-1+\beta}(D)} &\leq C\|Aw\|_{L^2(D)} = C\|(A - zI + zI)R(z; A)v\|_{L^2(D)} \\ &\leq C(\|v\|_{L^2(D)} + |z|\|w\|_{L^2(D)}) \leq C\|v\|_{L^2(D)}.\end{aligned}$$

It follows from this and (4.5) that

$$|z|\|e\|_{L^2(D)}^2 + \|e\|_{\tilde{H}^{\alpha/2}(D)}^2 \leq Ch^{\alpha/2-1+\beta}\|v\|_{L^2(D)}(|z|^{1/2}\|e\|_{L^2(D)} + \|e\|_{\tilde{H}^{\alpha/2}(D)}),$$

i.e.,

$$(4.7) \quad |z|\|e\|_{L^2(D)}^2 + \|e\|_{\tilde{H}^{\alpha/2}(D)}^2 \leq Ch^{\alpha-2+2\beta}\|v\|_{L^2(D)}^2,$$

from which follows directly the $\tilde{H}^{\alpha/2}(D)$ -norm of the error e . Next we deduce the $L^2(D)$ -norm of the error e by a duality argument: given $\varphi \in L^2(D)$, we define ψ and ψ_h , respectively, by

$$\psi = R(z; A^*)\varphi \quad \text{and} \quad \psi_h = R(z; A_h^*)P_h\varphi.$$

Then by duality

$$\|e\|_{L^2(D)} \leq \sup_{\varphi \in L^2(D)} \frac{|(e, \varphi)|}{\|\varphi\|_{L^2(D)}} = \sup_{\varphi \in L^2(D)} \frac{|z(e, \psi) - A(e, \psi)|}{\|\varphi\|_{L^2(D)}}.$$

Meanwhile it follows from (4.4) and (4.7) that

$$\begin{aligned}|z(e, \psi) - A(e, \psi)| &= |z(e, \psi - \psi_h) - A(e, \psi - \psi_h)| \\ &\leq |z|\|e\|_{L^2(D)}\|\psi - \psi_h\|_{L^2(D)} + C\|e\|_{\tilde{H}^{\alpha/2}(D)}\|\psi - \psi_h\|_{\tilde{H}^{\alpha/2}(D)} \\ &\leq Ch^{\alpha-2+2\beta}\|v\|_{L^2(D)}\|\varphi\|_{L^2(D)}.\end{aligned}$$

This completes the proof of the lemma. \square

Now we can state our first error estimate.

THEOREM 4.3. *Let u and u_h be solutions of problems (3.1) and (4.1) with $v \in L^2(D)$ and $v_h = P_h v$, respectively. Then for $t > 0$, there holds for any $\beta \in [1 - \alpha/2, 1/2)$*

$$\|u(t) - u_h(t)\|_{L^2(D)} + h^{\alpha/2-1+\beta}\|u(t) - u_h(t)\|_{\tilde{H}^{\alpha/2}(D)} \leq Ch^{\alpha-2+2\beta}t^{-1}\|v\|_{L^2(D)}.$$

Proof. Note the error $e(t) := u(t) - u_h(t)$ can be represented as

$$e(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{-zt}(w - w_h) dz,$$

where the contour $\Gamma = \{z : z = \rho e^{\pm i\delta_1}, \rho \geq 0\}$, and $w = R(z; A)v$ and $w_h = R(z; A_h)P_h v$. By Lemma 4.2, we have

$$\begin{aligned}\|e(t)\|_{\tilde{H}^{\alpha/2}(D)} &\leq C \int_{\Gamma} |e^{-zt}| \|w - w_h\|_{\tilde{H}^{\alpha/2}(D)} dz \\ &\leq Ch^{\alpha/2-1+\beta}\|v\|_{L^2(D)} \int_0^{\infty} e^{-\rho t \cos \delta_1} d\rho \leq Ch^{\alpha/2-1+\beta}t^{-1}\|v\|_{L^2(D)}.\end{aligned}$$

A similar argument yields the $L^2(D)$ -estimate. \square

4.2. Error estimate for smooth initial data. Next we turn to the case of smooth initial data, i.e., $v \in D(A)$. In order to obtain a uniform bound of the error, we employ an alternative integral representation. With $v_h = R_h v$, then there holds

$$\begin{aligned} u(t) - u_h(t) &= \int_{\Gamma} e^{-zt} (R(z; A)v - R(z; A_h)R_h v) dz \\ &= \int_{\Gamma_{\delta_1}^t} e^{-zt} (R(z; A)v - R(z; A_h)R_h v) dz, \end{aligned}$$

where $\Gamma_{\delta_1}^t = \Gamma_1 \cup \Gamma_2 \cup \Gamma_t$, $\Gamma_1 = \{z : z = \rho e^{i\delta_1}, \rho \geq t^{-1}\}$, $\Gamma_2 = \{z : z = \rho e^{-i\delta_1}, \rho \geq t^{-1}\}$, and $\Gamma_t = \{z : z = t^{-1} e^{i\theta}, \delta_1 \leq |\theta| \leq \pi\}$; cf. Figure 1(b). Then using the identities

$$R(z; A) = AA^{-1}R(z; A) = A(z^{-1}R(z; A) + z^{-1}A^{-1}) = z^{-1}R(z; A)A + z^{-1}I$$

the error $u(t) - u_h(t)$ can be represented as

$$(4.8) \quad u(t) - u_h(t) = \int_{\Gamma_{\delta_1}^t} z^{-1} e^{-zt} ((w - w_h) + (v - R_h v)) dz,$$

where $w = R(z; A)Av$ and $w_h = R(z; A_h)A_h R_h v$.

LEMMA 4.4. *For any $\varphi \in \tilde{H}^{\alpha/2}(D)$ and $z \in \Gamma_{\delta_1}^t$, there holds*

$$|z| \|\varphi\|_{L^2(D)}^2 + \|\varphi\|_{\tilde{H}^{\alpha/2}(D)}^2 \leq C|z| \|\varphi\|_{L^2(D)}^2 - A(\varphi, \varphi).$$

Proof. Note that $\Gamma_1 \cup \Gamma_2 \subset \Gamma$; thus it suffices to consider Γ_t . Set $z_t = t^{-1} e^{i\delta_1}$; then it is obvious that for $z \in \Gamma_t$ and $\varphi \in \tilde{H}^{\alpha/2}(D)$ we have $\text{dist}(z, \Sigma_\varphi) \geq \text{dist}(z_t, \Sigma_\varphi)$; cf. Figure 1(b). Thus the argument in proving (4.2) yields the desired result. \square

REMARK 4.1. For $v \in L^2(D)$, $z \in \Gamma_t$, let $w = R(z; A)v$ and $w_h = R(z; A_h)P_h v$. Then the arguments in Lemmas 4.2 and 4.4 yield the estimate (4.3).

THEOREM 4.5. *Let u and u_h be solutions of problems (3.1) and (4.1) with $v \in D(A)$ and $v_h = R_h v$, respectively. Then for any $\beta \in [1 - \alpha, 1/2)$, there holds*

$$\|u(t) - u_h(t)\|_{L^2(D)} + h^{\alpha/2-1+\beta} \|u(t) - u_h(t)\|_{\tilde{H}^{\alpha/2}(D)} \leq Ch^{\alpha-2+2\beta} \|Av\|_{L^2(D)}.$$

Proof. Let $w = R(z; A)Av$ and $w_h = R(z; A_h)A_h R_h v$. Together with the identity $A_h R_h = P_h A$ and Remark 4.1 gives

$$\|w_h - w\|_{L^2(D)} + h^{\alpha/2-1+\beta} \|w_h - w\|_{\tilde{H}^{\alpha/2}(D)} \leq Ch^{\alpha-2+2\beta} \|Av\|_{L^2(D)}.$$

Now it follows from this, the representation (4.8), and Lemma 2.4 that

$$\begin{aligned} \|u(t) - u_h(t)\|_{\tilde{H}^{\alpha/2}(D)} &\leq C \int_{\Gamma_{\delta_1}^t} |z^{-1}| e^{-\text{Re} zt} (\|w - w_h\|_{\tilde{H}^{\alpha/2}(D)} + \|v - R_h v\|_{\tilde{H}^{\alpha/2}(D)}) dz \\ &\leq Ch^{\alpha/2-1+\beta} \|Av\|_{L^2(D)} \int_{\Gamma_{\delta_1}^t} |z^{-1}| e^{-\text{Re} zt} dz. \end{aligned}$$

It suffices to bound the integral term. First we note that

$$\int_{\Gamma_1} |z^{-1}| e^{-\text{Re} zt} dz = \int_{t^{-1}}^{\infty} \rho^{-1} e^{-\rho t \cos \delta_1} d\rho \leq \int_{\cos \delta_1}^{\infty} x^{-1} e^{-x} dx \leq C,$$

which is also valid for the integral on the curve Γ_2 . Further, we have

$$\int_{\Gamma_t} |z^{-1}| |e^{-zt}| dz = \int_{\delta_1}^{2\pi-\delta_1} e^{\cos \theta} d\theta \leq C.$$

Hence we obtain the $\tilde{H}^{\alpha/2}(D)$ -estimate. The $L^2(D)$ -estimate follows analogously. \square

5. Error analysis for fully discrete schemes. Now we turn to error estimates for fully discrete schemes, obtained with either the backward Euler method or the (damped) Crank–Nicolson method in time.

5.1. Backward Euler method. We first consider the backward Euler method for approximating the first-order time derivative: for $n = 1, 2, \dots, N$

$$U^n - U^{n-1} + \tau A_h U^n = 0$$

with $U^0 = v_h$ which is an approximation of the initial data v . Then

$$(5.1) \quad U^n = (I + \tau A_h)^{-n} v_h, \quad U^0 = v_h, \quad n = 1, 2, \dots, N.$$

By the standard energy method, the backward Euler method is unconditionally stable, i.e., for any $n \in \mathbb{N}$, $\|(I + \tau A_h)^{-n}\| \leq 1$.

To analyze the scheme (5.1), we need the following smoothing property [5].

LEMMA 5.1. *For $n \in \mathbb{N}$, $n \geq 1$, $\gamma > 0$, and $s > 0$, there exists a constant $C > 0$, depending on γ only, such that*

$$(5.2) \quad \|A_h^\gamma (I + sA_h)^{-n}\| \leq C n^{-\gamma} s^{-\gamma}.$$

Proof. Let $r(z) = 1/(1+z)$. Then by [19, Lemma 9.2], for an arbitrary $R > 1$ and $\theta \in (0, \pi/2)$, there exist constants $c, C > 0$, and $\epsilon \in (0, 1)$ such that

$$(5.3) \quad |r(z)| \leq \begin{cases} e^{C|z|} & \forall |z| \leq \epsilon, \\ e^{-c|z|} & \forall |z| \leq R, |\arg z| \leq \theta. \end{cases}$$

Clearly, (5.2) is equivalent to $\|(nsA_h)^\gamma r(sA_h)^n\| \leq C$. The fact that A_h is sectorial implies that sA_h , $s > 0$, is also sectorial on X_h . Hence it suffices to show $\|(nA_h)^\gamma r(A_h)^n\| \leq C$. Let $F_n(z) = (nz)^\gamma r(z)^n$. Since $r(\infty) = 0$, by Lemma 3.5 and Remark 3.1

$$F_n(A_h) = \frac{1}{2\pi i} \int_{\Gamma_{\epsilon/n} \cup \Gamma_{\epsilon/n}^R \cup \Gamma^R} F_n(z) R(z; A_h) dz.$$

First, by (5.3), we deduce that for $z \in \Gamma_{\epsilon/n}$

$$|F_n(z)| \leq (n|z|)^\gamma e^{cn|z|} = \epsilon^\gamma e^{c\epsilon} \leq C.$$

Thus we have

$$\left\| \frac{1}{2\pi i} \int_{\Gamma_{\epsilon/n}} F_n(z) R(z; A_h) dz \right\| \leq C \frac{\epsilon}{n} \sup_{z \in \Gamma_{\epsilon/n}} \|R(z; A_h)\| \leq C.$$

Next, we note

$$\begin{aligned} \left\| \frac{1}{2\pi i} \int_{\Gamma_{\epsilon/n}^R} F_n(z)R(z; A_h) dz \right\| &\leq C \int_{\epsilon/n}^R (n\rho)^\gamma e^{-cn\rho} \rho^{-1} d\rho \\ &\leq C \int_{\epsilon}^{nR} \rho^{\gamma-1} e^{-\rho} d\rho \leq C \int_0^\infty \rho^{\gamma-1} e^{-\rho} d\rho \leq C. \end{aligned}$$

Last, there holds $|r(z)| \leq C|z|^{-1}$ for $z \in \Gamma^R$. Hence

$$|F_n(z)| \leq Cn^\gamma R^{\gamma-n} \leq C \quad \forall n \geq 1, \quad z \in \Gamma^R.$$

Thus we have the following bound for the integral on the curve Γ^R :

$$\left\| \frac{1}{2\pi i} \int_{\Gamma^R} F_n(z)R(z; A_h) dz \right\| \leq CR \sup_{z \in \Gamma^R} \|R(z; A_h)\| \leq C. \quad \square$$

Now we derive an error estimate for the fully discrete scheme (5.1) in case of smooth initial data, i.e., $v \in D(A)$.

THEOREM 5.2. *Let u and U^n be solutions of problems (3.1) and (5.1) with $v \in D(A)$ and $U^0 = R_h v$, respectively. Then for $t_n = n\tau$ and any $\beta \in [1 - \alpha/2, 1/2)$, there holds*

$$\|u(t_n) - U^n\|_{L^2(D)} \leq C(h^{\alpha-2+2\beta} + \tau)\|Av\|_{L^2(D)}.$$

Proof. Note that the error $e^n = u(t_n) - U^n$ can be split into

$$e^n = (u(t_n) - u_h(t_n)) + (u_h(t_n) - U^n) := \tilde{\varrho}^n + \tilde{\vartheta}^n,$$

where u_h denotes the semidiscrete Galerkin solution with $v_h = R_h v$. By Theorem 4.5, the term $\tilde{\varrho}^n$ satisfies the following estimate:

$$\|\tilde{\varrho}^n\|_{L^2(D)} \leq Ch^{\alpha-2+2\beta}\|Av\|_{L^2(D)}.$$

Next we bound the term $\tilde{\vartheta}^n$. Note that for $n \geq 1$,

$$\begin{aligned} (5.4) \quad \tilde{\vartheta}^n &= E_h(n\tau)v_h - (I + \tau A_h)^{-n}v_h \\ &= - \int_0^\tau \frac{d}{ds} (E_h(n(\tau - s))(I + sA_h)^{-n}v_h) ds \\ &= - \int_0^\tau nsA_h^2 E_h(n(\tau - s))(I + sA_h)^{-n-1}v_h ds. \end{aligned}$$

Then by Lemmas 3.4 and 5.1 we have

$$\begin{aligned} \|\tilde{\vartheta}^n\|_{L^2(D)} &\leq Cn^{1/2} \int_0^\tau s(\tau - s)^{-1/2} \|A_h^{3/2}(I + sA_h)^{-n-1}R_h v\|_{L^2(D)} ds \\ &\leq Cn^{1/2} \int_0^\tau s^{1/2}(n + 1)^{-1/2}(\tau - s)^{-1/2} \|A_h R_h v\|_{L^2(D)} ds \\ &\leq C\tau \|A_h R_h v\|_{L^2(D)}. \end{aligned}$$

The desired result follows from the identity $A_h R_h = P_h A$ and the $L^2(D)$ -stability of the projection P_h . \square

Next we give an error estimate for nonsmooth initial data $v \in L^2(D)$.

THEOREM 5.3. *Let u and U^n be solutions of problems (3.1) and (5.1) with $v \in L^2(D)$ and $U^0 = P_h v$, respectively. Then for $t_n = n\tau$ and any $\beta \in [1 - \alpha/2, 1/2)$, there holds*

$$\|u(t_n) - U^n\|_{L^2(D)} \leq C(h^{\alpha-2+2\beta} + \tau)t_n^{-1} \|v\|_{L^2(D)}.$$

Proof. Like before, we split the error $e^n = u(t_n) - U^n$ into

$$(5.5) \quad e^n = (u(t_n) - u_h(t_n)) + (u_h(t_n) - U^n) := \tilde{\varrho}^n + \tilde{\vartheta}^n,$$

where u_h denotes the semidiscrete Galerkin solution with $v_h = P_h v$. In view of Theorem 4.3, it remains to estimate the term $\tilde{\vartheta}^n$. By identity (5.4) and Lemmas 5.1 and 3.4, we have for $n \geq 1$

$$\begin{aligned} \|\tilde{\vartheta}^n\|_{L^2(D)} &\leq Cn \int_0^\tau s \|A_h^{3/2}(I + sA_h)^{-n-1} A_h^{1/2} E_h(n(\tau - s)) P_h v\|_{L^2(D)} ds \\ &\leq Cn \int_0^\tau s s^{-3/2} (n+1)^{-3/2} \|A_h^{1/2} E_h(n(\tau - s)) P_h v\|_{L^2(D)} ds \\ &\leq Cn^{-1/2} \int_0^\tau s^{-1/2} n^{-1/2} (\tau - s)^{-1/2} \|P_h v\|_{L^2(D)} ds \leq C\tau t_n^{-1} \|v\|_{L^2(D)}. \end{aligned}$$

The desired estimate now follows by the triangle inequality. \square

5.2. Crank–Nicolson method. Now we turn to the fully discrete scheme based on the Crank–Nicolson method. It reads

$$U^n - U^{n-1} + \tau A_h U^{n-1/2} = 0, \quad U^0 = v_h, \quad n = 1, 2, \dots, N,$$

where $U^{n-1/2} = (U^n + U^{n-1})/2$. Therefore we have

$$(5.6) \quad U^n = \left(I + \frac{\tau}{2} A_h\right)^{-n} \left(I - \frac{\tau}{2} A_h\right)^n v_h, \quad n = 1, 2, \dots, N.$$

It can be verified by the energy method that the Crank–Nicolson method is unconditionally stable, i.e., for any $n \in \mathbb{N}$, $\|(I + \frac{\tau}{2} A_h)^{-n} (I - \frac{\tau}{2} A_h)^n\| \leq 1$.

For the error analysis, we need a result on the rational function $r_{cn}(z) = (1 - z/2)/(1 + z/2)$.

LEMMA 5.4. *For any arbitrary $R > 0$, there exist $C > 0$ and $c > 0$ such that*

$$|e^{-nz} - r_{cn}(z)^n| \leq \begin{cases} C e^{-\frac{cn}{|z|}}, & |\arg z| \leq \delta_1, |z| \geq R, \\ Cn|z|^3 e^{-cn|z|}, & |\arg z| \leq \delta_1, |z| \leq R, \end{cases}$$

Proof. The proof of general cases can be found in [19, Lemmas 9.2 and 9.4]. We briefly sketch the proof here. By setting $w = 1/z$, the first inequality follows from

$$r_{cn}(z) = \frac{1 - z/2}{1 + z/2} = -\frac{1 - 2w}{1 + 2w} = -r(4w) = -e^{-4w + O(w^2)}, \quad w \rightarrow 0,$$

and that for $c \leq \cos \delta_1$,

$$|e^{-z} - r_{cn}(z)^n| \leq e^{-c|z|} \leq C e^{-\frac{c}{|z|}}, \quad |\arg z| \leq \delta_1, |z| \geq R.$$

The first estimate now follows by the triangle inequality. Meanwhile, we observe that

$$\begin{aligned} |r_{cn}(z) - e^{-z}| &\leq C|z|^3, \quad |\arg z| \leq \delta_1, \quad |z| \leq R, \\ |r_{cn}(z)| &\leq e^{-c|z|}, \quad |\arg z| \leq \delta_1, \quad |z| \leq R. \end{aligned}$$

Consequently, for z under consideration

$$|e^{-nz} - r_{cn}(z)^n| = \left| (e^{-z} - r_{cn}(z)) \sum_{j=0}^{n-1} r_{cn}(z)^j e^{-(n-1-j)z} \right| \leq C|z|^3 n e^{-cn|z|}. \quad \square$$

Now we can state an $L^2(D)$ -norm estimate for (5.6) in case of smooth initial data, i.e., $v \in D(A)$.

THEOREM 5.5. *Let u and U^n be solutions of problems (3.1) and (5.6) with $v \in D(A)$ and $U^0 = R_h v$, respectively. Then for $t_n = n\tau$ and any $\beta \in [1 - \alpha/2, 1/2)$, there holds*

$$\|u(t_n) - U^n\|_{L^2(D)} \leq C(h^{\alpha-2+2\beta} + \tau^2 t_n^{-1}) \|Av\|_{L^2(D)}.$$

Proof. Like before, we split the error e^n into

$$e^n = (u(t_n) - u_h(t_n)) + (u_h(t_n) - U^n) := \tilde{\varrho}^n + \tilde{\vartheta}^n,$$

where u_h denotes the semidiscrete Galerkin solution with $v_h = R_h v$. Then by Theorem 4.5, the term $\tilde{\varrho}^n$ satisfies the following estimate:

$$\|\tilde{\varrho}^n\|_{L^2(D)} \leq Ch^{\alpha-2+2\beta} \|Av\|_{L^2(D)}.$$

It remains to bound $\tilde{\vartheta}^n = E_h(n\tau)v_h - r_{cn}(\tau A_h)^n v_h$ by

$$\|\tilde{\vartheta}^n\|_{L^2(D)} \leq C\tau^2 t_n^{-1} \|A_h v_h\|_{L^2(D)}.$$

Note that τA_h is also sectorial, and further

$$\|(zI - \tau A_h)^{-1}\| = \tau^{-1} \|z/\tau - A_h\| \leq C|z|^{-1}.$$

With $t_n = n\tau$, it suffices to show

$$\|A_h^{-1}(E_h(n) - r_{cn}(A_h)^n)\| \leq Cn^{-1}.$$

By Lemma 3.5, there holds

$$A_h^{-1} r_{cn}(A_h)^n = \frac{1}{2\pi i} \int_{\Gamma_\epsilon \cup \Gamma_\epsilon^R \cup \Gamma^R} r_{cn}(z)^n z^{-1} R(z; A_h) dz.$$

Since $\|r_{cn}(z)^n z^{-1} R(z; A_h)\| = O(z^{-2})$ for large z , we can let R tend to ∞ . Further, by [19, Lemma 9.3], we have

$$A_h^{-1} E_h(n) = \frac{1}{2\pi i} \int_{\Gamma_\epsilon \cup \Gamma_\infty} e^{-nz} z^{-1} R(z; A_h) dz.$$

By Lemma 5.4,

$$\|(e^{-nz} - r_{cn}(z)^n) z^{-1} R(z; A_h)\| = O(z) \quad \text{as } z \rightarrow 0, \quad |\arg z| \leq \delta_1,$$

and consequently, by taking $\epsilon \rightarrow 0$, there holds

$$A_h^{-1}(E_h(n) - r_{cn}(A_h)^n) = \frac{1}{2\pi i} \int_{\Gamma} (e^{-nz} - r_{cn}(z)^n) z^{-1} R(z; A_h) dz,$$

where the contour Γ is given by $\Gamma = \{z : z = \rho e^{\pm i\delta_1}, \rho \geq 0\}$. By applying Lemma 5.4 with the parameter value $R = 1$, we deduce

(5.7)

$$\begin{aligned} \|A_h^{-1}(E_h(n) - r_{cn}(A_h)^n)\| &= \left\| \frac{1}{2\pi i} \int_{\Gamma} (e^{-nz} - r_{cn}(z)^n) z^{-1} R(z; A_h) dz \right\| \\ &\leq C \int_0^1 \rho n e^{-c n \rho} d\rho + C \int_1^{\infty} \rho^{-2} e^{-c n \rho^{-1}} d\rho \\ &\leq C n^{-1} \left(\int_0^{\infty} \rho e^{-\rho} d\rho + \int_0^{\infty} e^{-\rho} d\rho \right) \leq C n^{-1}. \quad \square \end{aligned}$$

Now we turn to the case of nonsmooth initial data, i.e., $v \in L^2(D)$. It is known that in case of the standard parabolic equation, the Crank–Nicolson method fails to give an optimal error estimate for such data unconditionally because of a lack of smoothing property [14, 20]. Hence we employ a damped Crank–Nicolson scheme, which is achieved by replacing the first two time steps by the backward Euler method. Further, we denote

$$(5.8) \quad r_{dcn}(z)^n = r_{bw}(z)^2 r_{cn}(z)^{n-2}.$$

The damped Crank–Nicolson scheme is also unconditionally stable. Further, the function $r_{dcn}(z)$ has the following estimates [7, Lemma 2.2].

LEMMA 5.6. *Let r_{dcn} be defined as in (5.8). Then there exist positive constants ϵ, R, C, c such that*

$$(5.9) \quad |r_{dcn}(z)^n| \leq \begin{cases} (1 + C|z|)^n, & |z| < \epsilon; \\ e^{-cn|z|}, & |z| \leq 1, |\arg(z)| \leq \delta_1; \\ C|z|^{-2} e^{-\frac{c(n-2)}{|z|}}, & |z| \geq 1, |\arg(z)| \leq \delta_1, n \geq 2; \\ C|z|^{-2}, & |z| \geq R, n \geq 2, \end{cases}$$

$$|r_{bw}(z)^2 - e^{-2z}| \leq C|z|^2, \quad |z| \leq \epsilon, \quad \text{or} \quad |\arg(z)| \leq \delta_1.$$

THEOREM 5.7. *Let u be the solution of problem (3.1), and $U^n = r_{dcn}(\tau A_h)^n U^0$ with $v \in L^2(D)$ and $U^0 = P_h v$. Then for $t_n = n\tau$ and any $\beta \in [1 - \alpha/2, 1/2)$, there holds*

$$\|u(t_n) - U^n\|_{L^2(D)} \leq C(h^{\alpha-2+2\beta} t_n^{-1} + \tau^2 t_n^{-2}) \|v\|_{L^2(D)}.$$

Proof. We split the error $e^n = u(t_n) - U^n$ as (5.5). Since the bound on $\tilde{\varrho}^n$ follows from Theorem 4.3, it remains to bound $\tilde{\vartheta}^n = E_h(\tau n)v_h - r_{dcn}(\tau A_h)^n v_h$ for $n \geq 1$ as

$$\|\tilde{\vartheta}^n\|_{L^2(D)} \leq C\tau^2 t_n^{-2} \|v_h\|_{L^2(D)}.$$

Let $F_n(z) = e^{-nz} - r_{dcn}(z)^n$. Then it suffices to show for $n \geq 1$

$$\|F_n(A_h)\| \leq Cn^{-2}.$$

The estimate is trivial for $n = 1, 2$ by boundedness. For $n > 2$, we split $F_n(z)$ into

$$F_n(z) = r_{bw}(z)^2(e^{-(n-2)z} - r_{cn}(z)^{n-2}) + e^{-(n-2)z}(e^{-2z} - r_{bw}(z)^2) \\ := f_1(z) + f_2(z).$$

It follows from Lemma 3.5 and [19, Lemma 9.3] that

$$r_{dcn}(A_h)^n = \frac{1}{2\pi i} \int_{\Gamma_\epsilon \cup \Gamma_\epsilon^R \cup \Gamma_\epsilon^R} r_{dcn}(z)^n R(z; A_h) dz, \\ E_h(n) = \frac{1}{2\pi i} \int_{\Gamma_\epsilon \cup \Gamma_\epsilon^\infty} e^{-nz} R(z; A_h) dz.$$

Using the fact $\|r_{dcn}(z)^n R(z; A_h)\| = O(z^{-3})$ as $z \rightarrow \infty$, we may let $R \rightarrow \infty$ to obtain

$$F_n(A_h) = \frac{1}{2\pi i} \int_{\Gamma_\epsilon \cup \Gamma_\epsilon^\infty} F_n(z) R(z; A_h) dz.$$

Further, by Lemma 5.6, $\|F_n(z) R(z; A_h)\| = O(z)$ as $z \rightarrow 0$, and consequently by taking $\epsilon \rightarrow 0$ and setting $\Gamma = \{z : z = \rho e^{\pm i\delta_1}, \rho \geq 0\}$, we have

$$(5.10) \quad F_n(A_h) = \frac{1}{2\pi i} \int_\Gamma F_n(z) R(z; A_h) dz \\ = \frac{1}{2\pi i} \int_\Gamma (f_1(z) + f_2(z)) R(z; A_h) dz.$$

Now we estimate the two terms separately. First, by Lemmas 5.4 and 5.6, we get

$$|f_1(z)| \leq |r_{dcn}(z)^n| + |r_{bw}(z)^2| |e^{-(n-2)z}| \leq C|z|^{-2} e^{-\frac{cn}{|z|}}, \quad z \in \Gamma, |z| \geq 1, \\ |f_1(z)| \leq |r_{bw}(z)^2| |r_{cn}(z)^{n-2} - e^{-(n-2)z}| \leq C|z|^3 n e^{-cn|z|}, \quad z \in \Gamma, |z| \leq 1.$$

Repeating the argument for (5.7) gives that for $n > 2$

$$\left\| \frac{1}{2\pi i} \int_\Gamma f_1(z) R(z; A_h) dz \right\| \leq Cn^{-2}.$$

As to the other term, we deduce from (5.9) that

$$|f_2(z)| \leq |e^{-(n-2)z}| |r_{bw}(z)^2 - e^{-2z}| \leq C|z|^2 \quad \forall |z| \leq \epsilon,$$

and thus we can change the integration path Γ to $\Gamma_{\epsilon/n}^\infty \cup \Gamma_{\epsilon/n}$. Further, we deduce from Lemma 5.6 that

$$|f_2(z)| = |e^{-(n-2)z}(r_{bw}(z)^2 - e^{-2z})| \leq C e^{-c(n-2)|z|} |z|^2 \quad \forall z \in \Gamma_{\epsilon/n}^\infty.$$

Thus, we derive the following bound for $n > 2$:

$$\left\| \frac{1}{2\pi i} \int_\Gamma f_1(z) R(z; A_h) dz \right\| \leq C \int_{\epsilon/n}^\infty e^{-c(n-2)\rho} \rho d\rho + C \int_{\Gamma_{\epsilon/n}} \rho d\rho \leq Cn^{-2}.$$

This completes the proof of the theorem. \square

6. Numerical results. In this section, we present numerical experiments to verify our theoretical results. To this end, we consider the following three examples:

- (a) smooth initial data: $v(x) = x(x-1)$, which lies in $\tilde{H}^{3/2-\epsilon}(D)$.
- (b) nonsmooth initial data:
 - (b1) $v(x) = \chi_{(1/2,1)}(x)$, the characteristic function of the interval $(1/2, 1)$;
 - (b2) $v(x) = x^{1/4}$;

Note that in (b1) $v \in \tilde{H}^{1/2-\epsilon}(D)$, while in (b2) $v \in \tilde{H}^{3/4-\epsilon}(D)$ for any $\epsilon \in (0, 1/4)$.

- (c) In this example, we consider the general case mentioned in Remark 2.3 with a discontinuous potential $q(x) = \chi_{(0,1/2)}(x)$, and $v(x) = \chi_{(1/2,1)}(x)$.

We examine separately the spatial and temporal convergence rates at $t = 1$. For the case of nonsmooth initial data, we are especially interested in the errors for t close to zero, and thus we also present the errors at $t = 0.1, 0.01, 0.005$, and 0.001 . The exact solutions to these examples are not available in closed form, and hence we compute the reference solution on a very refined mesh. We measure the accuracy of the numerical approximation U^n by the normalized errors $\|u(t_n) - U^n\|_{L^2(D)} / \|v\|_{L^2(D)}$ and $\|u(t_n) - U^n\|_{\tilde{H}^{\alpha/2}(D)} / \|v\|_{L^2(D)}$. The normalization enables us to observe the behavior of the errors with respect to time in case of nonsmooth initial data. The details of the computation of the stiffness matrix can be found in [11]. Since the bilinear form $a(\cdot, \cdot)$ induces an equivalent norm on $\tilde{H}^{\alpha/2}(D)$ (cf. (2.3)), we compute the $\tilde{H}^{\alpha/2}(D)$ -norm of the error by evaluating the bilinear form on a very refined mesh. To study the convergence rate in space, we use a time step size $\tau = 10^{-5}$ so that the time discretization error is negligible, and the space discretization error dominates.

6.1. Numerical results for example (a): Smooth initial data. In Table 1 we show the errors $\|u(t_n) - U^n\|_{L^2(D)}$ and $\|u(t_n) - U^n\|_{\tilde{H}^{\alpha/2}(D)}$ with the backward Euler method. We have set $\tau = 10^{-5}$ so that the error incurred by temporal discretization is negligible. In the table, **rate** refers to the convergence rate of the errors when the mesh size h (or time step size τ) halves, and the numbers in the bracket denote theoretical predictions. The numerical results show $O(h^{\alpha-1/2})$ and $O(h^{\alpha/2-1/2})$ convergence rates for the $L^2(D)$ - and $\tilde{H}^{\alpha/2}(D)$ -norms of the error, respectively. In Figure 2, we plot the results for $\alpha = 1.5$ at $t = 1$ in a log-log scale. The $\tilde{H}^{\alpha/2}(D)$ -norm estimate is fully confirmed, but the $L^2(D)$ -norm estimate is suboptimal: the empirical rate is one half order higher than the theoretical one. The suboptimality is attributed to the low regularity of the adjoint solution, used in Nitsche's trick. In view of the singularity of the term $x^{\alpha-1}$ in the solution representation (cf. Remark 2.1), the spatial discretization error is concentrated around the origin.

In Table 2, we let the spacial step size $h \rightarrow 0$ and examine the temporal convergence order, and we observe an $O(\tau)$ and $O(\tau^2)$ convergence rate for the backward

TABLE 1
 L^2 - and $\tilde{H}^{\alpha/2}$ -norms of the error for example (a), smooth initial data, with $\alpha = 1.25, 1.5, 1.75$ for backward Euler method and $\tau = 10^{-5}$.

α	h	1/16	1/32	1/64	1/128	1/256	1/512	Rate
1.25	L^2	5.13e-3	2.89e-3	1.69e-3	1.00e-3	6.03e-4	3.71e-4	≈ 0.76 (0.25)
	$\tilde{H}^{\alpha/2}$	4.93e-2	4.39e-2	3.98e-2	3.62e-2	3.29e-2	3.00e-2	≈ 0.14 (0.13)
1.5	L^2	3.62e-4	1.70e-4	8.37e-5	4.17e-5	2.09e-5	1.06e-5	≈ 1.02 (0.50)
	$\tilde{H}^{\alpha/2}$	7.57e-3	6.25e-3	5.20e-3	4.33e-3	3.58e-3	2.91e-3	≈ 0.27 (0.25)
1.75	L^2	1.12e-5	4.61e-6	1.92e-6	8.02e-7	3.35e-7	1.37e-7	≈ 1.26 (0.75)
	$\tilde{H}^{\alpha/2}$	4.63e-4	3.47e-4	2.58e-4	1.95e-4	1.46e-4	1.06e-4	≈ 0.42 (0.38)

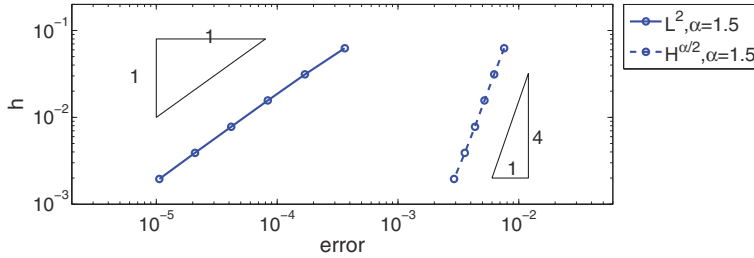


FIG. 2. Numerical results for example (a) (smooth data) with $\alpha = 1.5$ at $t = 1$.

TABLE 2

L^2 -norm of the error for example (a), smooth initial data, with $\alpha = 1.25, 1.5, 1.75, h = 2 \times 10^{-5}$ (BE = backward Euler; CN = Crank–Nicolson).

	τ	1/10	1/20	1/40	1/80	1/160	Rate
BE	$\alpha = 1.25$	3.01e-2	1.41e-2	6.63e-3	3.10e-3	1.41e-3	≈ 1.10 (1.00)
	$\alpha = 1.5$	1.32e-2	5.88e-3	2.71e-3	1.25e-3	5.62e-4	≈ 1.13 (1.00)
	$\alpha = 1.75$	4.79e-3	1.88e-3	7.95e-4	3.53e-4	1.55e-4	≈ 1.20 (1.00)
CN	$\alpha = 1.25$	3.18e-3	5.98e-4	1.35e-4	3.32e-5	8.52e-6	≈ 2.10 (2.00)
	$\alpha = 1.5$	3.22e-3	7.32e-4	1.75e-4	4.32e-5	1.05e-5	≈ 2.06 (2.00)
	$\alpha = 1.75$	3.67e-3	1.09e-3	3.33e-4	1.08e-4	3.09e-5	≈ 1.73 (-)

TABLE 3

L^2 -norm of the error for example (a), smooth initial data, for damped Crank–Nicolson method with $\alpha = 1.75$ and $h = 2 \times 10^{-5}$.

	τ	1/10	1/20	1/40	1/80	1/160	Rate
	$\alpha = 1.75$	7.57e-4	1.98e-4	5.45e-5	1.40e-5	2.90e-6	≈ 1.98 (2.00)

TABLE 4

L^2 - and $\tilde{H}^{\alpha/2}$ -norms of the error for example (b1), nonsmooth initial data, for backward Euler method with $\tau = 10^{-5}$.

α	h	1/16	1/32	1/64	1/128	1/256	1/512	Rate
1.25	L^2	6.65e-3	3.75e-3	2.18e-3	1.29e-3	7.78e-4	4.77e-4	≈ 0.76 (0.25)
	$H^{\alpha/2}$	6.36e-2	5.66e-2	5.12e-2	4.66e-2	4.24e-2	3.87e-2	≈ 0.14 (0.13)
1.5	L^2	3.78e-4	1.77e-4	8.56e-5	4.22e-5	2.09e-5	1.04e-5	≈ 1.03 (0.50)
	$H^{\alpha/2}$	7.31e-3	6.01e-3	5.00e-3	4.16e-3	3.43e-3	2.79e-3	≈ 0.27 (0.25)
1.75	L^2	2.11e-5	9.49e-6	4.06e-6	1.69e-6	6.83e-7	2.59e-7	≈ 1.27 (0.75)
	$H^{\alpha/2}$	3.63e-4	2.69e-4	1.99e-4	1.50e-4	1.12e-4	8.19e-5	≈ 0.43 (0.38)

Euler method and the Crank–Nicolson method, respectively. Note that for the case $\alpha = 1.75$, the Crank–Nicolson method fails to achieve an optimal convergence order. This is attributed to the fact that v is not in the domain of the differential operator ${}^R_0D_x^\alpha$ for $\alpha > 1.5$. In contrast, the damped Crank–Nicolson method yields the desired $O(\tau^2)$ convergence rate; cf. Table 3. This confirms the discussions in section 5.2.

6.2. Numerical results for nonsmooth initial data: Example (b).

In Tables 4, 5 and 6, we present numerical results for problem (b1). The results in Table 4 indicate that the spatial convergence rate is of the order $O(h^{\alpha-1+\beta})$ in the $L^2(D)$ -norm and $O(h^{\alpha/2-1+\beta})$ in the $\tilde{H}^{\alpha/2}(D)$ -norm, respectively, whereas the results in Table 5 show that the temporal convergence order is of order $O(\tau)$ and $O(\tau^2)$ for the backward Euler method and the damped Crank–Nicolson method, respectively.

TABLE 5
 L^2 -norm of the error for example (b1), nonsmooth initial data, with $h = 2 \times 10^{-5}$.

	τ	1/10	1/20	1/40	1/80	1/160	Rate
BE	$\alpha = 1.25$	3.73e-2	1.80e-2	8.53e-3	4.00e-3	1.81e-3	≈ 1.09 (1.00)
	$\alpha = 1.5$	1.26e-2	5.64e-3	2.59e-3	1.20e-3	5.40e-4	≈ 1.13 (1.00)
	$\alpha = 1.75$	3.68e-3	1.44e-3	6.12e-4	2.71e-4	1.20e-4	≈ 1.19 (1.00)
CN	$\alpha = 1.25$	3.52e-3	9.10e-4	2.39e-4	5.90e-5	1.30e-5	≈ 2.01 (2.00)
	$\alpha = 1.5$	8.86e-4	2.42e-4	6.46e-5	1.61e-5	3.44e-6	≈ 1.99 (2.00)
	$\alpha = 1.75$	1.86e-4	4.01e-5	1.02e-5	2.57e-6	5.41e-7	≈ 2.09 (2.00)

TABLE 6
 L^2 - and $\tilde{H}^{\alpha/2}$ -norms of the error for example (b1), nonsmooth initial data, with $\alpha = 1.5$ for backward Euler method and $\tau = 10^{-5}$.

t	h	1/16	1/32	1/64	1/128	1/256	1/512	Rate
0.1	L^2	3.64e-3	1.53e-3	7.42e-4	3.72e-5	1.87e-4	9.46e-5	≈ 1.04 (0.50)
	$\tilde{H}^{\alpha/2}$	7.00e-2	5.59e-2	4.62e-2	3.87e-2	3.21e-2	2.61e-2	≈ 0.28 (0.25)
0.01	L^2	2.81e-2	7.07e-2	1.63e-3	3.84e-4	9.21e-5	2.18e-5	≈ 2.07 (0.50)
	$\tilde{H}^{\alpha/2}$	4.04e-1	1.56e-1	6.09e-2	2.49e-2	1.03e-2	4.27e-3	≈ 1.31 (0.25)
0.005	L^2	4.27e-2	1.45e-2	3.44e-3	7.95e-4	1.88e-4	4.41e-4	≈ 2.07 (0.50)
	$\tilde{H}^{\alpha/2}$	5.94e-1	3.34e-1	1.27e-1	5.05e-2	2.08e-2	8.56e-3	≈ 1.26 (0.25)
0.001	L^2	1.41e-1	5.22e-2	1.64e-2	4.47e-3	1.02e-3	2.32e-3	≈ 1.80 (0.50)
	$\tilde{H}^{\alpha/2}$	2.61e0	1.45e0	6.63e-1	2.81e-1	1.08e-1	4.34e-2	≈ 1.20 (0.25)

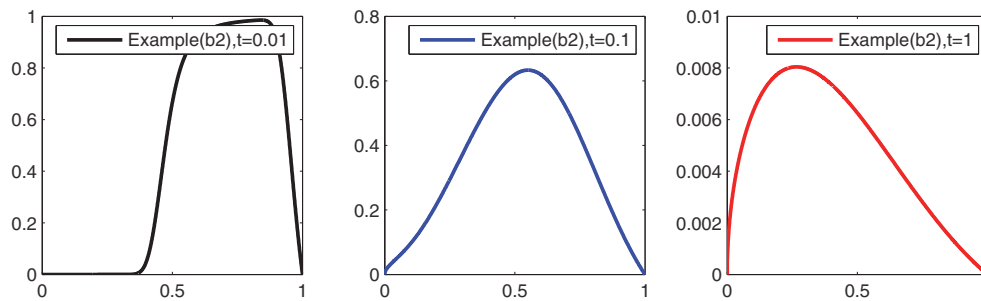


FIG. 3. Solution profile of example (b1) with $\alpha = 1.5$ at 0.01, 0.1, and 1.

For the case of nonsmooth initial data, we are interested in the errors for t closed to zero, and thus we check the error at $t = 0.1, 0.01, 0.005,$ and 0.001 . From Table 6, we observe that both the $L^2(D)$ -norm and the $\tilde{H}^{\alpha/2}(D)$ -norm of the error exhibit superconvergence, which theoretically remains to be established. Numerically, for this example, we note that the solution is smoother than in $\tilde{H}_L^{\alpha-1+\beta}(D)$ for small time t ; cf. Figure 3.

Similarly, the numerical results for problem (b2) are presented in Tables 7, 8, and 9; see also Figure 4 for a plot of the results in Table 9. The convergence is slower than that for example (b1), due to the lower solution regularity.

6.3. Numerical results for general problems: Example (c). Our theory can be easily extended to problems with a potential function $q \in L^\infty(D)$; cf. Remark 2.3. Garding's inequality holds for the bilinear form, and thus all theoretical results follow by the same argument. The normalized $L^2(D)$ - and $\tilde{H}^{\alpha/2}(D)$ -norms of the spatial error are shown in Table 10 at $t = 1$ for $\alpha = 1.25, 1.5,$ and 1.75 . The results concur with the preceding observations.

TABLE 7

L^2 - and $\tilde{H}^{\alpha/2}$ -norms of the error for example (b2), nonsmooth initial data, for backward Euler method with $\tau = 10^{-5}$.

α	h	1/16	1/32	1/64	1/128	1/256	1/512	Rate
1.25	L^2	6.31e-3	3.55e-3	2.07e-3	1.23e-3	7.38e-4	4.53e-4	≈ 0.76 (0.25)
	$H^{\alpha/2}$	6.03e-2	5.37e-2	4.86e-2	4.42e-2	4.02e-2	3.67e-2	≈ 0.14 (0.13)
1.5	L^2	4.11e-4	1.91e-4	9.24e-5	4.55e-5	2.26e-5	1.12e-5	≈ 1.03 (0.50)
	$H^{\alpha/2}$	7.88e-3	6.48e-3	5.39e-3	4.48e-3	3.70e-3	3.01e-3	≈ 0.27 (0.25)
1.75	L^2	2.75e-5	1.21e-6	5.09e-6	2.11e-6	8.48e-7	3.20e-7	≈ 1.28 (0.75)
	$H^{\alpha/2}$	4.50e-4	3.33e-4	2.46e-4	1.86e-4	1.39e-4	1.01e-4	≈ 0.42 (0.38)

TABLE 8

L^2 -norm of the error for example (b2), nonsmooth initial data, with $h = 2 \times 10^{-5}$.

	τ	1/10	1/20	1/40	1/80	1/160	Rate
BE	$\alpha = 1.25$	3.57e-2	1.71e-2	8.09e-3	3.80e-3	1.71e-3	≈ 1.09 (1.00)
	$\alpha = 1.5$	1.36e-2	6.82e-3	2.80e-3	1.30e-3	5.81e-4	≈ 1.13 (1.00)
	$\alpha = 1.75$	4.55e-3	1.78e-3	7.57e-4	3.35e-4	1.48e-4	≈ 1.20 (1.00)
CN	$\alpha = 1.25$	3.32e-3	8.59e-4	2.26e-4	5.60e-5	1.24e-5	≈ 2.03 (2.00)
	$\alpha = 1.5$	9.36e-4	2.59e-5	6.95e-5	1.74e-6	3.80e-7	≈ 1.99 (2.00)
	$\alpha = 1.75$	1.69e-4	4.43e-5	1.22e-5	3.15e-6	6.50e-7	≈ 1.99 (2.00)

TABLE 9

L^2 - and $\tilde{H}^{\alpha/2}$ -norms of the error for example (b2), nonsmooth initial data, for backward Euler method with $\tau = 10^{-5}$.

t	h	1/16	1/32	1/64	1/128	1/256	1/512	Rate
0.1	L^2	1.73e-2	8.56e-3	4.27e-3	2.14e-3	1.08e-3	5.43e-4	≈ 1.00 (0.50)
	$H^{\alpha/2}$	3.83e-1	3.20e-1	2.67e-1	2.23e-1	1.84e-1	1.50e-1	≈ 0.26 (0.25)
0.01	L^2	3.35e-2	1.39e-2	6.45e-3	3.17e-3	1.58e-3	7.97e-4	≈ 1.07 (0.50)
	$H^{\alpha/2}$	6.41e-1	4.89e-1	3.97e-1	3.28e-1	2.71e-1	2.20e-1	≈ 0.30 (0.25)
0.005	L^2	4.23e-2	1.83e-2	7.65e-3	3.61e-3	1.79e-3	8.96e-4	≈ 1.11 (0.50)
	$H^{\alpha/2}$	7.52e-1	5.89e-1	4.55e-1	3.71e-1	3.04e-1	2.47e-1	≈ 0.29 (0.25)
0.001	L^2	1.07e-1	4.12e-2	1.54e-2	5.89e-3	2.49e-3	1.19e-3	≈ 1.30 (0.50)
	$H^{\alpha/2}$	1.98e0	1.19e0	7.51e-1	5.19e-1	4.08e-1	3.28e-1	≈ 0.52 (0.25)

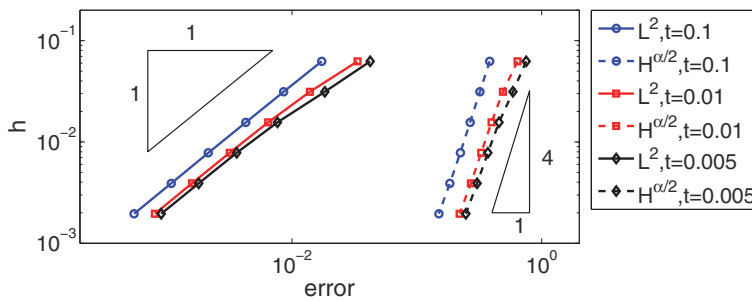


FIG. 4. Numerical results for example (b2) with $\alpha = 1.5$ at $t = 0.1, 0.01,$ and 0.005 .

7. Conclusion. In this paper, we have studied a Galerkin finite element method for an initial boundary value problem for the parabolic problem with a space fractional derivative of Riemann–Liouville type and order $\alpha \in (1, 2)$ using analytic semigroup theory. The existence and uniqueness of a weak solution in $L^2(0, T; \tilde{H}^{\alpha/2}(D))$ were established, and an improved regularity result was shown. Error estimates in the

TABLE 10

L^2 -norm of the error for example (c), nonsmooth initial data, example (c), with $\tau = 2 \times 10^{-5}$.

α	h	1/16	1/32	1/64	1/128	1/256	1/512	Rate
1.25	L^2	4.80e-3	2.71e-3	1.58e-3	9.40e-4	5.66e-4	3.48e-4	≈ 0.76 (0.25)
	$H^{\alpha/2}$	4.62e-2	4.12e-2	3.73e-2	3.39e-2	3.09e-2	2.82e-2	≈ 0.14 (0.13)
1.5	L^2	2.75e-4	1.31e-4	6.50e-5	3.24e-5	1.63e-5	8.20e-5	≈ 1.00 (0.50)
	$H^{\alpha/2}$	5.90e-3	6.86e-3	4.05e-3	3.37e-3	2.79e-3	2.26e-3	≈ 0.27 (0.25)
1.75	L^2	7.88e-6	3.19e-6	1.33e-6	5.58e-7	2.34e-7	9.60e-8	≈ 1.27 (0.75)
	$H^{\alpha/2}$	3.24e-4	2.42e-4	1.80e-4	1.36e-4	1.02e-4	7.43e-5	≈ 0.42 (0.38)

$L^2(D)$ - and the $\tilde{H}^{\alpha/2}(D)$ -norm were established for a space semidiscrete scheme with a piecewise linear finite element method, and $L^2(D)$ -norm estimates for fully discrete schemes based on the backward Euler method and (damped) Crank–Nicolson method, for both smooth and nonsmooth initial data.

The numerical experiments fully confirmed the convergence of the numerical schemes, but the $L^2(D)$ -norm error estimates are suboptimal: the empirical convergence rates are one-half order higher than the theoretical ones. This is attributed to the inefficiency of Nitsche’s trick, as a consequence of the low regularity of the adjoint solution. Numerically, we observe that the $\tilde{H}^{\alpha/2}(D)$ -norm convergence rates agree well with the theoretical ones. The optimal convergence rates in the $L^2(D)$ -norm and the $\tilde{H}^{\alpha/2}(D)$ -norm estimate for the fully discrete schemes still await theoretical justifications.

There are several avenues for future study. First, due to the inherent presence of the singular term $x^{\alpha-1}$ in the solution representation, the convergence of the standard finite element method is fairly slow. Hence it is of much interest to develop high-order schemes, e.g., based on singularity reconstruction technique and adaptively refined mesh. Second, our theory covers only the one-dimensional left-sided Riemann–Liouville derivative operator. Despite its popularity, some applications require more complex models, e.g., a variable diffusion coefficient and a multidimensional model. The variable coefficient can take different forms, e.g., ${}_0^R D_x^{\alpha-1}(\sigma u')$ or $(\sigma {}_0^R D_x^{\alpha-1} u)'$, with $\alpha \in (1, 2)$ and σ being the diffusion coefficient. The extension of our theory to these interesting cases remains elusive, since their solution theory is yet to be developed.

Appendix A. Proof of Theorem 3.1.

Proof. We divide the proof into four steps.

Step (i) (energy estimates for u_m). Upon taking u_m as the test function, the identity $2(u'_m, u_m) = \frac{d}{dt} \|u_m\|_{L^2(D)}^2$ for a.e. $0 \leq t \leq T$, and the coercivity of $A(\cdot, \cdot)$, we deduce

$$(A.1) \quad \frac{d}{dt} \|u_m(t)\|_{L^2(D)}^2 + c_0 \|u_m(t)\|_{\tilde{H}^{\alpha/2}(D)}^2 \leq 2 \|f(t)\|_{H^{-\alpha/2}(D)} \|u_m(t)\|_{\tilde{H}^{\alpha/2}(D)}.$$

Young’s inequality and integration in t over $(0, t)$ gives

$$\max_{0 \leq t \leq T} \|u_m(t)\|_{L^2(D)}^2 \leq \|v\|_{L^2(D)}^2 + C \|f\|_{L^2(0, T; H^{-\alpha/2}(D))}^2.$$

Next we integrate (A.1) from 0 to T and repeat the argument to get

$$(A.2) \quad \|u_m\|_{L^2(0, T; \tilde{H}^{\alpha/2}(D))}^2 \leq \|v\|_{L^2(D)}^2 + C \|f\|_{L^2(0, T; H^{-\alpha/2}(D))}^2.$$

Finally we bound $\|u'_m\|_{L^2(0, T; H^{-\alpha/2}(D))}$. For any $\varphi \in \tilde{H}^{\alpha/2}(D)$ such that $\|\varphi\|_{\tilde{H}^{\alpha/2}(D)} \leq 1$, we decompose it into $\varphi = P\varphi + (I - P)\varphi$ with $P\varphi \in \text{span}\{\omega_k\}_{k=1}^m$ and $I - P \in$

$\text{span}\{\omega_k\}_{k>m}$. By the stability of the projection P , $\|P\varphi\|_{\tilde{H}^{\alpha/2}(D)} \leq C\|\varphi\|_{\tilde{H}^{\alpha/2}(D)} \leq C$, it follows from $(u'_m, P\varphi) + A(u_m, P\varphi) = (f, P\varphi)$ and $(u'_m, P\varphi) = (u'_m, \varphi)$ that

$$|\langle u'_m(t), \varphi \rangle| = |\langle u'_m(t), P\varphi \rangle| \leq C(\|f(t)\|_{H^{-\alpha/2}(D)} + \|u_m(t)\|_{\tilde{H}^{\alpha/2}(D)}).$$

Consequently, by the duality argument and (A.2) we arrive at

$$(A.3) \quad \|u'_m\|_{L^2(0,T;H^{-\alpha/2}(D))}^2 \leq C(\|f\|_{L^2(0,T;H^{-\alpha/2}(D))}^2 + \|v\|_{L^2(D)}^2).$$

Step (ii) (convergent subsequence). By (A.2) and (A.3), there exists a subsequence, also denoted by $\{u_m\}$, and $u \in L^2(0, T; \tilde{H}^{\alpha/2}(D))$ and $\tilde{u} \in L^2(0, T; H^{-\alpha/2}(D))$, such that

$$(A.4) \quad \begin{aligned} u_m &\rightharpoonup u \quad \text{weakly in } L^2(0, T; \tilde{H}^{\alpha/2}(D)), \\ u'_m &\rightharpoonup \tilde{u} \quad \text{weakly in } L^2(0, T; H^{-\alpha/2}(D)). \end{aligned}$$

By choosing $\phi \in C_0^\infty[0, T]$ and $\psi \in \tilde{H}^{\alpha/2}(D)$, we deduce

$$\int_0^T \langle u'_m, \phi\psi \rangle dt = - \int_0^T \langle u_m, \phi'\psi \rangle dt.$$

By taking $m \rightarrow \infty$ we obtain

$$\int_0^T \langle \tilde{u}, \phi\psi \rangle dt = - \int_0^T \langle u, \phi'\psi \rangle dt = \int_0^T \langle u', \phi\psi \rangle dt.$$

Thus $\tilde{u} = u'$ by the density of $\{\phi(t)\psi(x)\}$ in $L^2(0, T; \tilde{H}^{\alpha/2}(D))$.

Step (iii) (weak form). Now for a fixed integer N , we choose a test function $\psi \in V_N = \text{span}\{\omega_k\}_{k=1}^N$, and $\phi \in C^\infty[0, T]$. Then for $m \geq N$, there holds

$$(A.5) \quad \int_0^T \langle u'_m, \psi\phi \rangle + A(u_m, \psi)\phi dt = \int_0^T \langle f, \psi\phi \rangle dt.$$

Then letting $m \rightarrow \infty$, (A.4) and the density of $\{\phi(t)\psi(x)\}$ in $L^2(0, T; \tilde{H}^{\alpha/2}(D))$ give

$$(A.6) \quad \int_0^T \langle u', \varphi \rangle + A(u, \varphi) dt = \int_0^T \langle f, \varphi \rangle dt \quad \forall \varphi \in L^2(0, T; \tilde{H}^{\alpha/2}(D)).$$

Consequently, we arrive at

$$\langle u', \varphi \rangle + A(u, \varphi) = \langle f, \varphi \rangle \quad \forall \varphi \in \tilde{H}^{\alpha/2}(D) \quad \text{a.e. } 0 \leq t \leq T.$$

Step (iv) (initial condition). The argument presented in [4, Theorem 3, p. 287] yields $u \in C([0, T]; L^2(D))$. By taking $\phi \in C^\infty[0, T]$ with $\varphi(T) = 0$ and $\psi \in \text{span}\{\omega_k\}_{k=1}^N$, integrating (A.5) and (A.6) by parts with respect to t , and a standard density argument, we arrive at the initial condition $u(0) = v$. The uniqueness follows directly from the energy estimates. \square

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REFERENCES

- [1] D. A. BENSON, S. W. WHEATCRAFT, AND M. M. MEERSCHAERT, *The fractional-order governing equation of Lévy motion*, Water Resources Res., 36 (2000), pp. 1413–1423.
- [2] V. J. ERVIN AND J. P. ROOP, *Variational formulation for the stationary fractional advection dispersion equation*, Numer. Methods Partial Differential Equations, 22 (2006), pp. 558–576.
- [3] V. J. ERVIN AND J. P. ROOP, *Variational solution of fractional advection dispersion equations on bounded domains in \mathbb{R}^d* , Numer. Methods Partial Differential Equations, 23 (2007), pp. 256–281.
- [4] L. C. EVANS, *Partial Differential Equations*, AMS, Providence, RI, 2010.
- [5] H. FUJITA AND A. MIZUTANI, *On the finite element method for parabolic equations. I. Approximation of holomorphic semi-groups*, J. Math. Soc. Japan, 28 (1976), pp. 749–771.
- [6] H. FUJITA AND T. SUZUKI, *Evolution Problems*, Handbook Numer. Anal. 2, North-Holland, Amsterdam, 1991, pp. 789–928.
- [7] A. HANSBO, *Nonsmooth data error estimates for damped single step methods for parabolic equations in Banach space*, Calcolo, 36 (1999), pp. 75–101.
- [8] M. HASSE, *The Functional Calculus for Sectorial Operators*, Birkhauser-Verlag, Basel, 2006.
- [9] Y. HATANO AND N. HATANO, *Dispersive transport of ions in column experiments: An explanation of long-tailed profiles*, Water Resources Res., 34 (1998), pp. 1027–1033.
- [10] K. ITO AND F. KAPPEL, *Evolutions Equations and Approximations*, Advances in Math. Appl. Sci. 16, World Scientific, River Edge, NJ, 2002.
- [11] B. JIN, R. LAZAROV, J. PASCIAK, AND W. RUNDELL, *A Finite Element Method for the Fractional Sturm-Liouville Problem*, preprint, arXiv:1307.5114, 2013.
- [12] B. JIN, R. LAZAROV, J. PASCIAK, AND W. RUNDELL, *Variational formulation of problems involving fractional order differential operators*, Math. Comp., in press.
- [13] A. A. KILBAS, H. M. SRIVASTAVA, AND J. J. TRUJILLO, *Theory and Applications of Fractional Differential Equations*, Elsevier, Amsterdam, 2006.
- [14] M. LUSKIN AND R. RANNACHER, *On the smoothing property of the Crank-Nicolson scheme*, Appl. Anal., 14 (1974), pp. 117–135.
- [15] R. METZLER AND J. KLAFTER, *The random walk's guide to anomalous diffusion: A fractional dynamics approach*, Phys. Rep., 339 (2000), pp. 1–77.
- [16] A. PAZY, *Semigroup of Linear Operators and Applications to Partial Differential Equations*, Springer-Verlag, New York, 1983.
- [17] C. TADJERAN AND M. M. MEERSCHAERT, *A second-order accurate numerical method for the two-dimensional fractional diffusion equation*, J. Comput. Phys., 220 (2007), pp. 813–823.
- [18] C. TADJERAN, M. M. MEERSCHAERT, AND H.-P. SCHEFFLER, *A second-order accurate numerical approximation for the fractional diffusion equation*, J. Comput. Phys., 213 (2006), pp. 205–213.
- [19] V. THOMÉE, *Galerkin Finite Element Methods for Parabolic Problems*, Springer-Verlag, Berlin, 2006.
- [20] M. ZLÁMAL, *Finite element methods for parabolic equations*, Math. Comp., 28 (1974), pp. 393–404.