IMA Journal of Numerical Analysis Advance Access published April 2, 2010

IMA Journal of Numerical Analysis Page 1 of 21
doi:10.1093/imanum/drp057

An implicit finite-difference time-stepping method for a sub-diffusion equation, with spatial discretization by finite elements

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[Received on 16 June 2009; revised on 13 December 2009]

The numerical solution for a class of sub-diffusion equations involving a parameter in the range $-1 < \alpha < 0$ is studied. For the time discretization, we use an implicit finite-difference Crank–Nicolson method and show that the error is of order $k^{2+\alpha}$, where k denotes the maximum time step. A nonuniform time step is employed to compensate for the singular behaviour of the exact solution at $t = 0$. We also consider a fully discrete scheme obtained by applying linear finite elements in space to the proposed time-stepping scheme. We prove that the additional error is of order $h^2 \max(1, \log k^{-1})$, where h is the parameter for the space mesh. Numerical experiments on some sample problems demonstrate our theoretical result.

Keywords: sub-diffusion (fractional diffusion); nonuniform time steps; finite-difference method; finite-element method.

1. Introduction

Consider an initial-value problem of the form

$$\partial_t u + \partial_t^{-\alpha} A u = f(t) \quad \text{for } 0 < t < T, \text{ with } u(0) = u_0, \tag{1.1}$$

for $-1 < \alpha < 0$ with ∂_t symbolizing the partial time differentiation and $\partial_t^{-\alpha}$ being the fractional time derivative that is defined through the Riemann–Liouville operator in Section 2. In applications, A is a linear, second-order elliptic partial differential operator in some spatial variable on some bounded domain. Typically, $A = -\nabla^2$. The problem (1.1) provides an anomalous slow diffusion (sub-diffusion) model, with u giving the probability density of the diffusing particles that have a mean-square displacement proportional to $t^{1+\alpha}$ ($\alpha + 1$ is the anomalous diffusion exponent) (see Balakrishnan, 1985; Wyss, 1986; Schneider & Wyss, 1989; Henry & Wearne, 2000; Metzler & Klafter, 2000; Yuste & Acedo, 2005). In the limiting case $\alpha = 0$ the problem (1.1) is reduced to a classical heat equation describing, for example, a microscopic model, where u represents the density of the diffusion particles that undergo Brownian motion with a mean-square displacement proportional to t.

For $0 < \alpha < 1$ the numerical solution of problem (1.1) has been extensively studied over the last two decades and a variety of numerical methods have been employed. For the finite-difference (FD) time discretization combined with standard finite elements (FEs) for the spatial discretization, we refer to the work of McLean *et al.* (1996) and McLean & Mustapha (2007) and related references therein. The orthogonal spline collocation and mixed FEs have been investigated by Yan & Fairweather (1992),

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Fairweather (1994) and Pani & Fairweather (2002). For the time convolution quadrature approach combined with linear FEs in space, see Cuesta *et al.* (2006). For the discontinuous Galerkin (DG) in time and the FEs in space, we refer to the recent work of Mustapha & McLean (2009). López-Fernández & Palencia (2004) and McLean & Thomée (2004) analysed an alternative style of time discretization using the N-point quadrature rule in an approximate Laplace inversion formula.

Recently, McLean & Mustapha (2009) studied the piecewise-constant DG method for the time discretization of (1.1) in the case $-1 < \alpha < 0$. The scheme was essentially a modified implicit backward Euler method. An optimal order convergence rate of order k was proved, where k denoted the maximum time step. The space discretization by means of the piecewise-linear standard Galerkin method was also considered and an optimal order convergence was proved.

In this work the generalized Crank–Nicolson scheme for the time discretization of (1.1) is investigated. Formally, such a scheme is second-order accurate. However, it seems that, in the presence of a weakly singular kernel and a fractional derivative operator $\partial_t^{-\alpha}$, it is not possible to achieve such an order of accuracy. We show an $\mathcal{O}(k^{\alpha+2})$ convergence rate, where a family of nonuniform meshes based on concentrating the time steps near $t = 0$ is employed to compensate for the lack of smoothness of the solution u (near $t = 0$). In contrast, for $0 < \alpha < 1$, McLean & Mustapha (2007) applied a similar scheme and succeeded in showing an $\mathcal{O}(k^2)$ convergence rate. In this work we also address the space discretization by means of linear FEs. Indeed, estimating the error bounds from either time or space discretization of (1.1) for $-1 < \alpha < 0$ is more difficult compared to the case where $0 < \alpha < 1$. Finally, we demonstrate numerically that our error bounds are sharp.

Even though the case $-1 < \alpha < 0$ in problem (1.1) is of equal interest to the case $0 < \alpha < 1$, it has received less attention from the numerical point of view. For a brief history on the numerical solution of (1.1) for $-1 < \alpha < 0$ (in addition to McLean & Mustapha, 2009) we cite the following works. Langlands & Henry (2005) studied a scheme of implicit Euler type for (1.1), but with a different treatment of the fractional derivative and employing only uniform time steps. They provided a partial error analysis and presented numerical experiments indicating $\mathcal{O}(k^{1+\alpha})$ convergence when $\alpha = -1/2$. Their method also incorporated the usual second-order central FD approximation of $Au = -u_{xx}$, giving an additional error term of order h^2 for a uniform spatial step-size h. In comparison, Yuste & Acedo (2005) proposed and analysed an explicit FD method for the time and space discretizations of problem (1.1). An $\mathcal{O}(k + h^2)$ convergence result was shown, assuming that the exact solution of (1.1) is sufficiently smooth at $t = 0$. Cuesta *et al.* (2006) examined formally second-order accurate, convolution quadrature schemes for (1.1). They proved $\mathcal{O}(k^2)$ convergence for $0 < \alpha < 1$, but only $\mathcal{O}(k^{2+\alpha})$ convergence if $-1 < \alpha < 0$. Schädle *et al.* (2006) and López-Fernández *et al.* (2008) developed fast algorithms for evaluating convolution quadrature sums and for reducing the memory requirements of such methods. In contrast, for a sub-diffusion problem with a smooth kernel, a piecewise-linear DG time-stepping scheme was proposed and analyzed in my recent work Mustapha (2009), where an $\mathcal{O}(k^2)$ convergence rate was shown.

Another type of scheme involving Laplace transformation combined with a quadrature along a contour in the complex plane provides spectral accuracy for the time discretization but appears to offer little scope for handling nonlinear versions of (1.1) (see López-Fernández *et al.*, 2006; McLean & Thomée, 2009).

The following is an outline of the paper. In Section 2 the stability property of the exact solution of problem (1.1) is derived and the time-stepping scheme is defined by (2.7). Also, notation that is needed throughout the paper is introduced. In Section 3 the stability of the proposed scheme is proved using the methods of McLean *et al.* (1996). The error bound from the time discretization is derived in Section 4 (more precisely in Theorem 4.3). In Section 5 a spatially discrete version of (2.7) is described using piecewise-linear FEs, and we show that the additional error is $\mathcal{O}(h^2|\log k|)$, so that we achieve essentially an optimal accuracy in space. To relax our error analysis proofs, some technical lemmas will be addressed in the appendix. Finally, Section 6 presents some numerical studies of a few test problems.

2. Notation, assumptions and preliminary results

In this section we reformulate our initial boundary-value problem (1.1) in an abstract sense. We also define our numerical scheme for time discretization and introduce notation that is needed throughout the paper.

Assume that A is a positive-semidefinite, self-adjoint linear operator with a complete eigensystem $\phi_1, \phi_2, \phi_3, \ldots$ in a real Hilbert space $\mathbb{H}$. The solution u and source term f take values in $\mathbb{H}$, and the initial datum u_0 is an element of $\mathbb{H}$. We denote the norm of an element v in $\mathbb{H}$ by $\|v\|$ and assume the normalization $\|\phi_m\| = 1$. We let λ_m denote the eigenvalue corresponding to ϕ_m, i.e., $A\phi_m = \lambda_m \phi_m$, and assume the ordering $0 \leqslant \lambda_1 \leqslant \lambda_2 \leqslant \lambda_3 \leqslant \cdots$. Thus the associated bilinear form

$$A(u, v) = \langle Au, v\rangle = \sum_{m=1}^{\infty} \lambda_m \langle u, \phi_m\rangle\langle \phi_m, v\rangle \quad \text{for } u, v \in D(A^{1/2}) \tag{2.1}$$

is positive semi-definite. For instance, when $\mathbb{H} = L_2(\Omega)$ for a bounded, Lipschitz domain $\Omega \in \mathbb{R}^d$ and $A = -\nabla^2$ with homogeneous Dirichlet or Neumann boundary conditions, we have $A(u, v) = \int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}x$. Let

$$\omega_\alpha(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)} \quad \text{for } 0 < t < \infty \text{ and } 0 < \alpha < \infty,$$

and denote the Riemann–Liouville fractional integration operator of order α by

$$\mathfrak{D}_\alpha v(t) = \int_0^t \omega_\alpha(t-s)v(s)\mathrm{d}s \quad \text{for } 0 < t < \infty.$$

We extend this definition to obtain a fractional *derivative* by setting

$$\mathfrak{D}_\alpha v(t) = (\mathfrak{D}_{1+\alpha} v)'(t) = \frac{\partial}{\partial t}\int_0^t \omega_{\alpha+1}(t-s)Au(s)\mathrm{d}s \quad \text{for } -1 < \alpha < 0.$$

Setting $\partial_t^{-\alpha} = \mathfrak{D}_\alpha$ for $-1 < \alpha < 0$ in (1.1), our problem is to find u: $[0, T] \to \mathbb{H}$ satisfying

$$u' + \mathfrak{D}_\alpha(Au) = f(t) \quad \text{for } 0 < t < T, \text{ with } u(0) = u_0, \tag{2.2}$$

for a given initial datum $u_0 \in \mathbb{H}$ and inhomogeneous term $f \in L_1((0, T); \mathbb{H})$. Following the discussion given in McLean & Mustapha (2009, Section 2), we observe that

$$\int_0^T A(\mathfrak{D}_\alpha v(t), v(t))\mathrm{d}t \geqslant 0. \tag{2.3}$$

As a consequence of this, one may show (via an energy argument) that the abstract initial-value problem (2.2) admits a unique mild solution (see McLean *et al.*, 1996; McLean & Thomée, 2010) and that this solution is stable in the sense that

$$\|u(t)\| \leqslant \|u_0\| + 2\int_0^t \|f(s)\|\mathrm{d}s \quad \text{for } 0 \leqslant t \leqslant T. \tag{2.4}$$

Typically, we have positive constants M and σ such that the solution u of (2.2) satisfies

$$t^{1+\alpha}\|Au'(t)\| + t^{2+\alpha}\|Au''(t)\| \leqslant Mt^{\sigma-1} \quad \text{for } t > 0. \tag{2.5}$$

For instance, if $f \equiv 0$ and $u_0 \in D(A^r)$ for some $r > 0$ then (2.5) holds with $\sigma = (1+\alpha)r$ (see Cuesta *et al.*, 2006, equation (8.2); McLean & Thomée, 2010, Theorem 2.1). This type of regularity will eventually allow us to bound the error arising from the time discretization.

To discretize in time we introduce the grid points $0 = t_0 < t_1 < t_2 < \cdots < t_N = T$ and set

$$k_n = t_n - t_{n-1}, \quad k = \max_{1\leqslant n\leqslant N}(k_n) \quad \text{and} \quad t_{n-1/2} = \frac{1}{2}(t_{n-1}+t_n) \quad \text{for } 1 \leqslant n \leqslant N.$$

Furthermore, for a given function v defined on the time grid points t_n for $n \geqslant 0$, we set $v^n = v(t_n)$. By $\bar{v}$ we denote

$$\bar{v}(t) = \begin{cases} v^1 & \text{for } t_0 < t < t_1, \\ (v^{n-1}+v^n)/2 & \text{for } t_{n-1} < t < t_n \text{ and } 2 \leqslant n \leqslant N. \end{cases} \tag{2.6}$$

To define our numerical scheme, starting from an approximation $U^0 \approx u_0$ to the initial data, we consider a time discretization

$$U^n - U^{n-1} + \int_{t_{n-1}}^{t_n} \mathfrak{D}_\alpha(A\bar{U})(t)\mathrm{d}t = \int_{t_{n-1}}^{t_n} f(t)\mathrm{d}t =: \tilde{f}^n \quad \text{for } 1 \leqslant n \leqslant N \tag{2.7}$$

that generates an approximate solution $U^n \approx u(t_n)$.

The modification on the first subinterval ensures that $\bar{U}$ does not depend on U^0, which is necessary for our numerical scheme in the case $u_0 \notin D(A)$.

Integrating and using the definition of $\bar{U}$, we find that

$$\begin{aligned}
&\int_{t_{n-1}}^{t_n} \mathfrak{D}_\alpha(A\bar{U})(t)\mathrm{d}t \\
&\quad = \mathfrak{D}_{\alpha+1}(A\bar{U})(t_n) - \mathfrak{D}_{\alpha+1}(A\bar{U})(t_{n-1}) \\
&\quad = \sum_{j=1}^{n-1}\int_{t_{j-1}}^{t_j} [\omega_{\alpha+1}(t_n-s) - \omega_{\alpha+1}(t_{n-1}-s)]A\bar{U}(s)\mathrm{d}s + \int_{t_{n-1}}^{t_n} \omega_{\alpha+1}(t_n-s)A\bar{U}(s)\mathrm{d}s \\
&\quad = \omega_{n1}AU^1 + \frac{1}{2}\sum_{j=2}^{n-1}\omega_{nj}A(U^{j-1}+U^j) + \frac{1}{2}\omega_{nn}A(U^{n-1}+U^n),
\end{aligned}$$

where, for $1 \leqslant j \leqslant n-1$,

$$\omega_{nj} = \int_{t_{j-1}}^{t_j}[\omega_{\alpha+1}(t_n-s) - \omega_{\alpha+1}(t_{n-1}-s)]\mathrm{d}s \quad \text{and} \quad \omega_{nn} = \int_{t_{n-1}}^{t_n}\omega_{\alpha+1}(t_n-s)\mathrm{d}s = \omega_{\alpha+2}(k_n).$$

Therefore the approximate solution U^n for $n \geqslant 1$ can be computed as follows:

$$(I + \omega_{11}A)U^1 = U^0 + \tilde{f}^1, \tag{2.8}$$

and for $2 \leqslant n \leqslant N$ we have

$$(2I + \omega_{nn} A)U^n = (2I - \omega_{nn} A)U^{n-1} + 2\tilde{f}^n - 2\omega_{n1} AU^1 + \sum_{j=2}^{n-1} \omega_{nj} A(U^{j-1} + U^j), \tag{2.9}$$

where I denotes the identity operator on $\mathbb{H}$. So the scheme (2.7) is implicit.

As mentioned earlier, (2.7) is formally second-order accurate, but, for problems of the form (2.2) with $-1 < \alpha < 0$, our theoretical and numerical results demonstrate the infeasibility of getting convergence rates better than $\mathcal{O}(k^{2+\alpha})$. In comparison, for the case $0 < \alpha < 1$ (that is, we have a Riemann–Liouville fractional integral operator, and we deal with a sup-diffusion problem and not a sub-diffusion problem), an $\mathcal{O}(k^2)$ convergence rate has been proved for the time discretization scheme (2.7) (see McLean & Mustapha, 2007).

In practice, our chief interest is in a smoothly graded mesh of the form

$$t_n = (nk)^\gamma \quad \text{for } 0 \leqslant n \leqslant N, \text{ with } k = T^{1/\gamma}/N \text{ and } \gamma \geqslant 1. \tag{2.10}$$

By choosing $\gamma > 1$ we can make the time step-size k_n smaller near $t = 0$ and thereby compensate the singular behaviour of the solution of (2.2) as $t \downarrow 0$.

One can check that our graded mesh satisfies the following properties:

$$k_n \leqslant k_{n+1}, \quad k_n \leqslant \gamma k t_n^{1-1/\gamma} \text{ for } n \geqslant 1 \quad \text{and} \quad t_n \leqslant 2^\gamma t_{n-1} \text{ for } n \geqslant 2. \tag{2.11}$$

Throughout the paper, C denotes a generic constant that is independent of k and h (the time and spacial step-sizes, respectively) but may depend on T, σ, M, γ and α.

3. Stability of the numerical solution

In this section we prove the stability of our scheme (2.7) by adapting a proof from McLean *et al.* (1996, Lemma 4.1). We note that the scheme is unconditionally stable.

THEOREM 3.1. The discrete initial-value problem (2.7) has a unique solution $U^1, U^2, \ldots, U^n$ in $\mathbb{H}$. Furthermore,

$$U^n \in D(A) \quad \text{and} \quad \|U^n\| \leqslant \|U^0\| + 2\sum_{j=1}^{n} \|\tilde{f}^j\| \quad \text{for } 1 \leqslant n \leqslant N.$$

Proof. For $n = 1$ we take the inner product of both sides of (2.8) with the eigenfunction ϕ_m and see that the Fourier coefficients of U^1 are uniquely determined from those of U^0 and $\tilde{f}^1$ as follows:

$$U_m^1 = \frac{U_m^0 + \tilde{f}_m^1}{1 + \omega_{11}\lambda_m}.$$

To see why $U^1 \in D(A)$ we note that

$$\|AU^1\|^2 = \sum_{m=1}^{\infty} \left(\lambda_m U_m^1\right)^2 = \sum_{m=1}^{\infty} \left(\frac{\lambda_m}{1 + \omega_{11}\lambda_m}\right)^2 \left(U_m^0 + \tilde{f}_m^1\right)^2 \leqslant \omega_{11}^{-2} \sum_{m=1}^{\infty} \left(U_m^0 + \tilde{f}_m^1\right)^2,$$

so that $\|AU^1\| \leqslant \omega_{11}^{-1}\|U^0 + \tilde{f}^1\|$.

A simple induction on $n \geqslant 2$ gives the existence of a unique $U^1, U^2, \ldots, U^n$ satisfying (2.7). In fact, we see from (2.9) that the Fourier coefficients of U^n are given by

$$U_m^n = \frac{1}{2+\omega_{nn}\lambda_m}\left\{(2-\omega_{nn}\lambda_m)U_m^{n-1} + 2\tilde{f}_m^n - \lambda_m\left(2\omega_{n1}U_m^1 + \sum_{j=2}^{n-1}\omega_{nj}(U_m^{j-1}+U_m^j)\right)\right\},$$

from which we also see by induction on n that $U^n \in D(A)$.

It now remains to prove the stability estimate. We set $n = 1$ in (2.7) and take the inner product of both sides with $2U^1$ to obtain

$$2\|U^1\|^2 - 2\langle U^1, U^0\rangle + 2\int_0^{t_1}\langle \mathfrak{D}_\alpha(A\bar{U})(t), \bar{U}(t)\rangle \mathrm{d}t = 2\langle U^1, \tilde{f}^1\rangle.$$

Since $\|U^1 - U^0\|^2 = \|U^1\|^2 - 2\langle U^1, U^0\rangle + \|U^0\|^2$, it follows that

$$\|U^1\|^2 - \|U^0\|^2 + \|U^1 - U^0\|^2 + 2\int_0^{t_1}\langle \mathfrak{D}_\alpha(A\bar{U})(t), \bar{U}(t)\rangle \mathrm{d}t = 2\langle U^1, \tilde{f}^1\rangle, \tag{3.1}$$

and, because $\|U^1 - U^0\|^2 + 2\int_0^{t_1}\langle \mathfrak{D}_\alpha(A\bar{U})(t), \bar{U}(t)\rangle \mathrm{d}t \geqslant 0$, we find

$$\begin{aligned}(\|U^1\| + \|U^0\|)(\|U^1\| - \|U^0\|) = \|U^1\|^2 - \|U^0\|^2 &\leqslant 2\langle U^1, \tilde{f}^1\rangle \\ &\leqslant 2\|U^1\|\|\tilde{f}^1\| \leqslant 2(\|U^1\| + \|U^0\|)\|\tilde{f}^1\|,\end{aligned}$$

so that $\|U^1\| - \|U^0\| \leqslant 2\|\tilde{f}^1\|$, as required.

For $n \geqslant 2$ we take the inner product of both sides of (2.7) with $U^n + U^{n-1}$ to obtain

$$\|U^n\|^2 - \|U^{n-1}\|^2 + 2\int_{t_{n-1}}^{t_n}\langle \mathfrak{D}_\alpha(A\bar{U})(t), \bar{U}(t)\rangle \mathrm{d}t = \langle U^n + U^{n-1}, \tilde{f}^n\rangle.$$

Let $\|U^{n^*}\| = \max_{0\leqslant n\leqslant N}\|U^n\|$. Summing the above equation from $n = 2$ to $n = n^*$ gives

$$\|U^{n^*}\|^2 - \|U^1\|^2 + 2\int_{t_1}^{t_{n^*}}\langle \mathfrak{D}_\alpha(A\bar{U})(t), \bar{U}(t)\rangle \mathrm{d}t = \sum_{n=2}^{n^*}\langle U^n + U^{n-1}, \tilde{f}^n\rangle.$$

Adding this equation to (3.1), we see that

$$\|U^{n^*}\|^2 - \|U^0\|^2 + 2\int_0^{t_{n^*}}\langle \mathfrak{D}_\alpha(A\bar{U})(t), \bar{U}(t)\rangle \mathrm{d}t \leqslant 2\|U^1\|\|\tilde{f}^1\| + \sum_{n=2}^{n^*}\|U^n + U^{n-1}\|\|\tilde{f}^n\|.$$

Since $\int_0^{t_{n^*}}\langle \mathfrak{D}_\alpha(A\bar{U})(t), \bar{U}(t)\rangle \mathrm{d}t \geqslant 0$ and $\|U^{n^*}\| = \max_{0\leqslant n\leqslant N}\|U^n\|$, it follows that

$$\|U^{n^*}\|^2 \leqslant \|U^0\|^2 + 2\|U^{n^*}\|\sum_{n=1}^{n^*}\|\tilde{f}^n\| \leqslant \|U^{n^*}\|\left(\|U^0\| + 2\sum_{n=1}^{N}\|\tilde{f}^n\|\right),$$

so that $\|U^{n^*}\| \leqslant \|U^0\| + 2\sum_{n=1}^{N}\|\tilde{f}^n\|$. Because $\|U^{n^*}\| = \max_{0\leqslant n\leqslant N}\|U^n\|$, the proof is completed. □

4. Error bound from the time discretization

In this section we estimate the error $e^n = U^n - u(t_n)$ when U^n is given by (2.7) and u is the exact solution of (2.2). Some ideas from McLean & Mustapha (2007, Section 3) are used.

Integrating (2.2) from $t = t_{n-1}$ to $t = t_n$ shows that the exact solution u satisfies

$$u(t_n) - u(t_{n-1}) + \int_{t_{n-1}}^{t_n} \mathfrak{D}_\alpha(Au)(t)\mathrm{d}t = \tilde{f}^n.$$

Comparing this with (2.7), we observe that the error e^n satisfies

$$e^n - e^{n-1} + \int_{t_{n-1}}^{t_n} \mathfrak{D}_\alpha(A\bar{e})(t)\mathrm{d}t = \eta^{n-1/2}, \tag{4.1}$$

where

$$\eta^{n-1/2} = \int_{t_{n-1}}^{t_n} \mathfrak{D}_\alpha(Au - A\bar{u})(t)\mathrm{d}t. \tag{4.2}$$

Since (4.1) has the same form as (2.7), and, since $e^0 = U^0 - u_0$, the stability result of Theorem 3.1 implies that

$$\|e^n\| \leqslant \|U^0 - u_0\| + 2\sum_{j=1}^{n} \|\eta^{j-1/2}\| \quad \text{for } 1 \leqslant n \leqslant N. \tag{4.3}$$

Thus our task is reduced to estimating the sum on the right-hand side of this inequality.

One can show that

$$u(t) - \bar{u}(t) = \widehat{e}_1(t) + \widehat{e}_2(t) \quad \text{for } t_{n-1} < t < t_n \text{ with } 2 \leqslant n \leqslant N,$$

where

$$\widehat{e}_1(t) = \frac{1}{2}\int_t^{t_n}\int_s^{t_n} u''(q)\mathrm{d}q\,\mathrm{d}s - \frac{1}{2}\int_{t_{n-1}}^{t}\int_s^{t_n} u''(q)\mathrm{d}q\,\mathrm{d}s \quad \text{and} \quad \widehat{e}_2(t) = (t - t_{n-1/2})u'(t_n).$$

For $0 < t < t_1$ we set $\widehat{e}_1(t) = u(t) - \bar{u}(t)$ and $\widehat{e}_2(t) = 0$.

Using this, we make the splitting $\eta^{j-1/2} = \eta_1^{j-1/2} + \eta_2^{j-1/2}$, where

$$\eta_1^{j-1/2} = \int_{t_{j-1}}^{t_j} \mathfrak{D}_\alpha(A\widehat{e}_1)(t)\mathrm{d}t \quad \text{and} \quad \eta_2^{j-1/2} = \int_{t_{j-1}}^{t_j} \mathfrak{D}_\alpha(A\widehat{e}_2)(t)\mathrm{d}t. \tag{4.4}$$

In the next two lemmas we bound the terms $\sum_{j=1}^n \|\eta_1^{j-1/2}\|$ and $\sum_{j=1}^n \|\eta_2^{j-1/2}\|$.

LEMMA 4.1 For $\eta_1^{j-1/2}$ defined as in (4.4) we have

$$\sum_{j=1}^{n} \|\eta_1^{j-1/2}\| \leqslant C\left(\int_0^{t_1} t^{1+\alpha}\|Au'(t)\|\mathrm{d}t + \sum_{j=2}^{n} k_j^{2+\alpha}\int_{t_{j-1}}^{t_j} \|Au''(t)\|\mathrm{d}t\right).$$

Proof. Integrating and splitting, we have

$$\eta_1^{j-1/2} = \mathfrak{D}_{\alpha+1}(A\widehat{e}_1)(t_j) - \mathfrak{D}_{\alpha+1}(A\widehat{e}_1)(t_{j-1})$$
$$= \sum_{i=1}^{j-1}\int_{t_{i-1}}^{t_i}[\omega_{\alpha+1}(t_j-s)-\omega_{\alpha+1}(t_{j-1}-s)]A\widehat{e}_1(s)\mathrm{d}s + \int_{t_{j-1}}^{t_j}\omega_{\alpha+1}(t_j-s)A\widehat{e}_1(s)\mathrm{d}s.$$

For $j=1$ we have $0<s<t_1$ and then

$$A\widehat{e}_1(s) = Au(s) - Au(t_1) = -\int_s^{t_1} Au'(\xi)\mathrm{d}\xi.$$

Using this and changing the order of integrals, we have

$$\|\eta_1^{1/2}\| \leqslant \int_0^{t_1}\omega_{\alpha+1}(t_1-s)\|A\widehat{e}_1(s)\|\mathrm{d}s \leqslant \int_0^{t_1}\omega_{\alpha+1}(t_1-s)\int_s^{t_1}\|Au'(\xi)\|\mathrm{d}\xi\,\mathrm{d}s$$
$$= \int_0^{t_1}\|Au'(\xi)\|\int_0^{\xi}\omega_{\alpha+1}(t_1-s)\mathrm{d}s\,\mathrm{d}\xi \leqslant \int_0^{t_1}\omega_{\alpha+2}(\xi)\|Au'(\xi)\|\mathrm{d}\xi, \tag{4.5}$$

where in the last inequality we used the fact that

$$\int_0^{\xi}\omega_{\alpha+1}(t_1-s)\mathrm{d}s = \omega_{\alpha+2}(t_1) - \omega_{\alpha+2}(t_1-\xi) \leqslant \omega_{\alpha+2}(\xi).$$

For the sum of $\|\eta_1^{j-1/2}\|$ over $j\geqslant 2$, noting first that

$$\omega_{\alpha+1}(t_{j-1}-s) - \omega_{\alpha+1}(t_j-s) > 0$$

and hence changing the order of summation, we get

$$\sum_{j=2}^{n}\|\eta_1^{j-1/2}\| \leqslant \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\int_{t_{i-1}}^{t_i}[\omega_{\alpha+1}(t_{j-1}-s)-\omega_{\alpha+1}(t_j-s)]\|A\widehat{e}_1(s)\|\mathrm{d}s$$
$$+\sum_{j=2}^{n}\int_{t_{j-1}}^{t_j}\omega_{\alpha+1}(t_j-s)\|A\widehat{e}_1(s)\|\mathrm{d}s$$
$$= \sum_{i=1}^{n-1}\int_{t_{i-1}}^{t_i}[\omega_{\alpha+1}(t_i-s)-\omega_{\alpha+1}(t_n-s)]\|A\widehat{e}_1(s)\|\mathrm{d}s$$
$$+\sum_{j=2}^{n}\int_{t_{j-1}}^{t_j}\omega_{\alpha+1}(t_j-s)\|A\widehat{e}_1(s)\|\mathrm{d}s$$
$$\leqslant \int_0^{t_1}\omega_{\alpha+1}(t_1-s)\|A\widehat{e}_1(s)\|\mathrm{d}s + 2\sum_{j=2}^{n}\int_{t_{j-1}}^{t_j}\omega_{\alpha+1}(t_j-s)\|A\widehat{e}_1(s)\|\mathrm{d}s.$$

Using the definition of $\widehat{e}_1$, we observe that

$$\|A\widehat{e}_1(s)\| \leqslant k_j \int_{t_{j-1}}^{t_j} \|Au''(q)\| \mathrm{d}q \quad \text{for } t_{j-1} < s < t_j \text{ with } j \geqslant 2,$$

and thus we have

$$\sum_{j=2}^{n} \|\eta_1^{j-1/2}\| \leqslant \int_0^{t_1} \omega_{\alpha+1}(t_1 - s)\|A\widehat{e}_1(s)\| \mathrm{d}s + 2\sum_{j=2}^{n} k_j \omega_{\alpha+2}(k_j) \int_{t_{j-1}}^{t_j} \|Au''(q)\| \mathrm{d}q.$$

From (4.5) we have

$$\int_0^{t_1} \omega_{\alpha+1}(t_1 - s)\|A\widehat{e}_1(s)\| \mathrm{d}s \leqslant \int_0^{t_1} \omega_{\alpha+2}(\xi)\|Au'(\xi)\| \mathrm{d}\xi$$

and therefore the proof is complete. □

$$\mathbf{K}_\alpha^{i,j} = \frac{-\alpha}{2\Gamma(\alpha+1)} \int_{t_{i-1}}^{t_i} (s - t_{i-1})(t_i - s)(t_j - s)^{\alpha-1} \,\mathrm{d}s \quad \text{for } 1 \leqslant i \leqslant j \leqslant N.$$

An integration by parts yields that

$$\mathbf{K}_\alpha^{j,j} = \frac{-\alpha}{2\Gamma(\alpha+1)} \int_{t_{j-1}}^{t_j} (s - t_{j-1})(t_j - s)^{\alpha} \,\mathrm{d}s$$

$$= \frac{-\alpha}{2\Gamma(\alpha+2)} \int_{t_{j-1}}^{t_j} (t_j - s)^{\alpha+1} \,\mathrm{d}s = -\frac{\alpha}{2}\omega_{\alpha+3}(k_j), \tag{4.6}$$

and, since $k_j \geqslant k_{j-1}$, we have

$$\mathbf{K}_\alpha^{j,j} - \mathbf{K}_\alpha^{j-1,j-1} = -\frac{\alpha}{2}(\omega_{\alpha+3}(k_j) - \omega_{\alpha+3}(k_{j-1})) \geqslant 0. \tag{4.7}$$

In the next lemma we derive the bound of $\sum_{j=1}^{n} \|\eta_2^{j-1/2}\|$. For the sake of briefness we introduce the following additional notation:

LEMMA 4.2 For $\eta_2^{j-1/2}$ defined as in (4.4) we have

$$\sum_{j=2}^{n} \|\eta_2^{j-1/2}\| \leqslant C \left(\sum_{i=2,n} k_i^{2+\alpha} \|Au'(t_i)\| + k_n^{2+\alpha} \|Au'(t_n)\| \right.$$
$$\left. + \sum_{j=2}^{n} k_j^{2+\alpha} \int_{t_{j-1}}^{t_j} \|Au''(s)\| \mathrm{d}s + \sum_{j=3}^{n} k_j^{1+\alpha} (k_j - k_{j-1}) \|Au'(t_{j-1})\| \right).$$

Proof. First, observe that $\eta_2^{1/2} = 0$. For $j \geqslant 2$, integrating and splitting, we obtain

$$\eta_2^{j-1/2} = \mathfrak{D}_{\alpha+1}(A\widehat{e}_2)(t_j) - \mathfrak{D}_{\alpha+1}(A\widehat{e}_2)(t_{j-1})$$
$$= \sum_{i=2}^{j} Au'(t_i) \int_{t_{i-1}}^{t_i} (s - t_{i-1/2})\omega_{\alpha+1}(t_j - s)\mathrm{d}s$$
$$- \sum_{i=2}^{j-1} Au'(t_i) \int_{t_{i-1}}^{t_i} (s - t_{i-1/2})\omega_{\alpha+1}(t_{j-1} - s)\mathrm{d}s.$$

The use of the identity $2(s - t_{i-1/2}) = -((s - t_{i-1})(t_i - s))'$ followed by an integration by parts shows that, for $1 \leqslant i \leqslant j$, we have

$$\int_{t_{i-1}}^{t_i} (s - t_{i-1/2})\omega_{\alpha+1}(t_j - s)\mathrm{d}s = \frac{-\alpha}{2\Gamma(\alpha+1)} \int_{t_{i-1}}^{t_i} (s - t_{i-1})(t_i - s)(t_j - s)^{\alpha-1}\,\mathrm{d}s = \mathbf{K}_\alpha^{i,j}. \quad (4.8)$$

Similarly, for $1 \leqslant i \leqslant j-1$ we have

$$\int_{t_{i-1}}^{t_i} (s - t_{i-1/2})\omega_{\alpha+1}(t_{j-1} - s)\mathrm{d}s = \mathbf{K}_\alpha^{i,j-1}.$$

Thus $\eta_2^{j-1/2} = \eta_{21}^{j-1/2} + \eta_{22}^{j-1/2}$, where

$$\eta_{21}^{j-1/2} = Au'(t_j)\mathbf{K}^{j,j} - Au'(t_{j-1})\mathbf{K}^{j-1,j-1} \quad (4.9)$$

and

$$\eta_{22}^{j-1/2} = \sum_{i=2}^{j-1} Au'(t_i)\mathbf{K}_\alpha^{i,j} - \sum_{i=2}^{j-2} Au'(t_i)\mathbf{K}_\alpha^{i,j-1}. \quad (4.10)$$

To estimate (4.9), adding and subtracting $Au'(t_{j-1})$ and using (4.7), we obtain

$$\|\eta_{21}^{j-1/2}\| \leqslant \|Au'(t_j) - Au'(t_{j-1})\|\mathbf{K}^{j,j} + \|Au'(t_{j-1})\|(\mathbf{K}^{j,j} - \mathbf{K}^{j-1,j-1}).$$

Since $\|Au'(t_{j-1})\|\mathbf{K}^{j,j} \leqslant \|Au'(t_{j-1}) - Au'(t_j)\|\mathbf{K}^{j,j} + \|Au'(t_j)\|\mathbf{K}^{j,j}$, we have

$$\|\eta_{21}^{j-1/2}\| \leqslant 2\|Au'(t_j) - Au'(t_{j-1})\|\mathbf{K}^{j,j} + \|Au'(t_j)\|\mathbf{K}^{j,j} - \|Au'(t_{j-1})\|\mathbf{K}^{j-1,j-1},$$

and hence

$$\sum_{j=2}^{n} \|\eta_{21}^{j-1/2}\| \leqslant 2\sum_{j=2}^{n} \|Au'(t_{j-1}) - Au'(t_j)\|\mathbf{K}^{j,j} + \|Au'(t_n)\|\mathbf{K}^{n,n} - \|Au'(t_1)\|\mathbf{K}^{1,1}.$$

Now the use of

$$Au'(t_j) - Au'(t_{j-1}) = \int_{t_{j-1}}^{t_j} Au''(q)\mathrm{d}q \quad \text{for } j \geqslant 1 \quad (4.11)$$

and (4.6) yields that

$$\sum_{j=2}^{n}\|\eta_{21}^{j-1/2}\| \leqslant -\alpha\sum_{j=2}^{n}\omega_{\alpha+3}(k_j)\int_{t_{j-1}}^{t_j}\|Au''(s)\|\mathrm{d}s - \frac{\alpha}{2}\|Au'(t_n)\|\omega_{\alpha+3}(k_n). \tag{4.12}$$

To estimate $\eta_{22}^{j-1/2}$ in (4.10), note first that $\eta_{22}^{3/2}=0$. For $j\geqslant 3$ we make the splitting $\eta_{22}^{j-1/2} = \eta_{221}^{j-1/2}+\eta_{222}^{j-1/2}$, where

$$\eta_{221}^{j-1/2} = Au'(t_2)\mathbf{K}_\alpha^{2,j} + \sum_{i=3}^{j-1}\left(Au'(t_i) - \frac{k_{i-1}^3}{k_i^3}Au'(t_{i-1})\right)\mathbf{K}_\alpha^{i,j},$$

$$\eta_{222}^{j-1/2} = -\sum_{i=3}^{j-1}Au'(t_{i-1})\left(\mathbf{K}_\alpha^{i-1,j-1} - \frac{k_{i-1}^3}{k_i^3}\mathbf{K}_\alpha^{i,j}\right). \tag{4.13}$$

For the first of these quantities, changing the order of summation, we have

$$\sum_{j=3}^{n}\|\eta_{221}^{j-1/2}\| \leqslant \sum_{j=3}^{n}\|Au'(t_2)\|\mathbf{K}_\alpha^{2,j} + \sum_{j=3}^{n}\sum_{i=3}^{j-1}\|Au'(t_i) - Au'(t_{i-1})k_{i-1}^3/k_i^3\|\mathbf{K}_\alpha^{i,j}$$

$$= \|Au'(t_2)\|\sum_{j=3}^{n}\mathbf{K}_\alpha^{2,j} + \sum_{i=3}^{n-1}\|Au'(t_i) - Au'(t_{i-1})k_{i-1}^3/k_i^3\|\sum_{j=i+1}^{n}\mathbf{K}_\alpha^{i,j}. \tag{4.14}$$

Changing the order of summation and using Lemma A.1 implies that

$$\sum_{j=3}^{n}\|\eta_{222}^{j-1/2}\| \leqslant \sum_{i=3}^{n-1}\|Au'(t_{i-1})\|\sum_{j=i+1}^{n}\left(\mathbf{K}_\alpha^{i-1,j-1} - \frac{k_{i-1}^3}{k_i^3}\mathbf{K}_\alpha^{i,j}\right),$$

and a shift of the indices gives

$$\sum_{j=3}^{n}\|\eta_{222}^{j-1/2}\| \leqslant \sum_{i=2}^{n-2}\|Au'(t_i)\|\sum_{j=i+1}^{n-1}\mathbf{K}_\alpha^{i,j} - \sum_{i=3}^{n-1}\|Au'(t_{i-1})\|\frac{k_{i-1}^3}{k_i^3}\sum_{j=i+1}^{n}\mathbf{K}_\alpha^{i,j}.$$

Hence, using $|\|Au'(t_i)\| - \|Au'(t_{i-1})\|k_{i-1}^3/k_i^3| \leqslant \|Au'(t_i) - Au'(t_{i-1})k_{i-1}^3/k_i^3\|$, we observe that

$$\sum_{j=3}^{n}\|\eta_{222}^{j-1/2}\| \leqslant \|Au'(t_2)\|\sum_{j=3}^{n-1}\mathbf{K}_\alpha^{2,j} + \sum_{i=3}^{n-1}\|Au'(t_i) - Au'(t_{i-1})k_{i-1}^3/k_i^3\|\sum_{j=i+1}^{n}\mathbf{K}_\alpha^{i,j}. \tag{4.15}$$

To proceed in our proof we add and subtract $Au'(t_{i-1})$ and then use (4.11) and the inequality $1 - k_{i-1}^3/k_i^3 \leqslant 3k_i^{-1}(k_i - k_{i-1})$ to reach

$$\|Au'(t_i) - Au'(t_{i-1})k_{i-1}^3/k_i^3\| \leqslant \|Au'(t_i) - Au'(t_{i-1})\| + \|Au'(t_{i-1})\|(1 - k_{i-1}^3/k_i^3)$$

$$\leqslant \int_{t_{i-1}}^{t_i}\|Au''(q)\|\mathrm{d}q + 3k_i^{-1}(k_i - k_{i-1})\|Au'(t_{i-1})\|. \tag{4.16}$$

Therefore, combining the estimates from (4.13)–(4.15), and with the help of Lemma A.2 and (4.16), we find that

$$\sum_{j=2}^{n}\|\eta_{22}^{j-1/2}\| \leqslant k_2\omega_{\alpha+2}(k_2)\|Au'(t_2)\| + \sum_{i=3}^{n-1}\omega_{\alpha+2}(k_i)\left(k_i\int_{t_{i-1}}^{t_i}\|Au''(s)\|\mathrm{d}s + 3(k_i-k_{i-1})\|Au'(t_{i-1})\|\right).$$

Using $\eta_2^{j-1/2}=\eta_{21}^{j-1/2}+\eta_{22}^{j-1/2}$, (4.12) and the last inequality, we complete the proof. □

In the next theorem the error estimate from our time discretization scheme (2.7) is derived. Mainly, we combine the results of Lemmas 4.1 and 4.2 and then show how the convergence rate depends on the mesh grading parameter $\gamma \geqslant 1$.

THEOREM 4.3. Let u be the solution of the initial-value problem (2.2) and let U^n be the solution of the discrete-time scheme (2.7). Then, for $1\leqslant n\leqslant N$, we have

$$\|U^n-u(t_n)\| \leqslant \|U^0-u_0\| + C\times\begin{cases} k^{\gamma\sigma} & \text{if } 1\leqslant\gamma<(2+\alpha)/\sigma,\\ k^{2+\alpha}\log(t_n/t_1) & \text{if } \gamma=(2+\alpha)/\sigma,\\ k^{2+\alpha} & \text{if } \gamma>(2+\alpha)/\sigma.\end{cases}$$

Proof. Using (4.3), $\eta^{j-1/2}=\eta_1^{j-1/2}+\eta_2^{j-1/2}$ and Lemmas 4.1 and 4.2, we obtain the following bound:

$$\begin{aligned}\|U^n-u(t_n)\| &\leqslant \|U^0-u_0\|\\ &\quad + C\left(\int_0^{t_1} t^{1+\alpha}\|Au'(t)\|\mathrm{d}t + k_2^{2+\alpha}\|Au'(t_2)\| + k_n^{2+\alpha}\|Au'(t_n)\|\right.\\ &\quad\left. + \sum_{j=2}^{n}k_j^{2+\alpha}\int_{t_{j-1}}^{t_j}\|Au''(t)\|\mathrm{d}t + \sum_{j=3}^{n}k_j^{1+\alpha}(k_j-k_{j-1})\|Au'(t_{j-1})\|\right). \quad (4.17)\end{aligned}$$

Using $k_j^{1+\alpha}\geqslant k_{j-1}^{1+\alpha}$ followed by adding and subtracting $Au'(t_j)$, we find that

$$\begin{aligned}k_j^{1+\alpha}(k_j-k_{j-1})\|Au'(t_{j-1})\| &\leqslant (k_j^{2+\alpha}-k_{j-1}^{2+\alpha})\|Au'(t_{j-1})\|\\ &\leqslant k_j^{2+\alpha}\|Au'(t_j)-Au'(t_{j-1})\| + k_j^{2+\alpha}\|Au'(t_j)\| - k_{j-1}^{2+\alpha}\|Au'(t_{j-1})\|,\end{aligned}$$

and hence, with the help of (4.11), we obtain

$$\sum_{j=3}^{n}k_j^{1+\alpha}(k_j-k_{j-1})\|Au'(t_{j-1})\| \leqslant \sum_{j=3}^{n}k_j^{2+\alpha}\int_{t_{j-1}}^{t_j}\|Au''(s)\|\mathrm{d}s + k_n^{2+\alpha}\|Au'(t_n)\| - k_2^{2+\alpha}\|Au'(t_2)\|.$$

Inserting this bound in (4.17) gives

$$\begin{aligned}\|U^n-u(t_n)\| &\leqslant \|U^0-u_0\|\\ &\quad + C\left(\int_0^{t_1} t^{1+\alpha}\|Au'(t)\|\mathrm{d}t + k_n^{2+\alpha}\|Au'(t_n)\| + \sum_{j=2}^{n}k_j^{2+\alpha}\int_{t_{j-1}}^{t_j}\|Au''(t)\|\mathrm{d}t\right). \quad (4.18)\end{aligned}$$

Using the regularity assumption on the exact solution given by (2.5), we have

$$\int_0^{t_1} t^{1+\alpha}\|Au'(t)\|\mathrm{d}t \leqslant M\int_0^{t_1} t^{\sigma-1}\,\mathrm{d}t = \frac{M}{\sigma}t_1^{\sigma} = \frac{M}{\sigma}k^{\gamma\sigma}. \tag{4.19}$$

The use of (2.5) and (2.11) implies that

$$\begin{aligned} k_n^{2+\alpha}\|Au'(t_n)\| &\leqslant Mk_n^{2+\alpha}t_n^{\sigma-2-\alpha} \leqslant Ck^{2+\alpha}t_n^{\sigma-(2+\alpha)/\gamma} \\ &\leqslant C\times\begin{cases} k^{2+\alpha}(nk)^{\gamma\sigma-(2+\alpha)} \leqslant k^{\gamma\sigma} & \text{if } \sigma < (2+\alpha)/\gamma, \\ k^{2+\alpha} & \text{if } \sigma \geqslant (2+\alpha)/\gamma, \end{cases} \end{aligned} \tag{4.20}$$

and

$$\begin{aligned} \sum_{j=2}^{n} k_j^{2+\alpha}\int_{t_{j-1}}^{t_j}\|Au''(t)\|\mathrm{d}t &\leqslant C\sum_{j=2}^{n} k_j^{2+\alpha}t_j^{\sigma-3-\alpha}k_j \leqslant Ck^{2+\alpha}\sum_{j=2}^{n} t_j^{\sigma-(2+\alpha)/\gamma-1}k_j \\ &\leqslant Ck^{2+\alpha}\int_{t_1}^{t_n} t^{\sigma-(2+\alpha)/\gamma-1}\,\mathrm{d}t \\ &\leqslant Ck^{2+\alpha}\times\begin{cases} t_1^{\sigma-(2+\alpha)/\gamma} & \text{if } \sigma < (2+\alpha)/\gamma, \\ \log(t_n/t_1) & \text{if } \sigma = (2+\alpha)/\gamma, \\ t_n^{\sigma-(2+\alpha)/\gamma} & \text{if } \sigma > (2+\alpha)/\gamma. \end{cases} \end{aligned} \tag{4.21}$$

Substituting $t_1^{\sigma-(2+\alpha)/\gamma} = k^{\sigma\gamma-(2+\alpha)}$ in the first case and then inserting (4.19)–(4.21) in (4.18), we obtain the desired result. □

5. Error estimate from the fully discrete scheme

In this section we propose our fully discrete scheme for solving (2.2) using FEs in space and Crank–Nicolson in time and derive the error bound. Assume that $\mathbb{H} = L_2(\Omega)$ for a bounded, convex, polyhedral domain Ω and that A is a strongly elliptic, second-order, self-adjoint linear partial differential operator.

For $r = 1, 2$ we define the real Hilbert space $\dot{H}^r$ with norm given by $\|v\|_{\dot{H}^r}^2 = \|v\|^2 + \|A^{r/2}v\|^2$ to be

$$\dot{H}^r = \{v \in H^r(\Omega)\colon v = 0 \text{ on } \partial\Omega\}$$

in the case of homogeneous Dirichlet boundary conditions, whereas for homogeneous Neumann boundary conditions we have

$$\dot{H}^1 = H^1(\Omega) \quad\text{and}\quad \dot{H}^2 = \{v \in H^2(\Omega)\colon \partial_n v = 0 \text{ on } \partial\Omega\}.$$

We triangulate Ω and define the usual continuous, piecewise-linear FE space $V_h \subseteq \dot{H}^1$, where h denotes the maximum diameter of the elements. Let the mesh be quasi-uniform so that the Ritz projector $R_h\colon \dot{H}^1 \to V_h$ for the modified (strictly positive-definite) operator $A + I$, given by

$$\mathsf{A}(R_h v, \chi) + \langle R_h v, \chi\rangle = \mathsf{A}(v, \chi) + \langle v, \chi\rangle \quad \text{for } v \in \dot{H}^1 \text{ and } \chi \in V_h,$$

has the approximation property

$$\|v - R_h v\| \leqslant Ch^2 \|v\|_{\dot{H}^2} \quad \text{for } v \in \dot{H}^2. \tag{5.1}$$

Using the bilinear form $\mathsf{A}(u, \chi)$ associated with A, we write the weak form of problem (2.2) as

$$\langle \partial_t u, \chi \rangle + \mathsf{A}(\mathfrak{D}_\alpha(Au)(t), \chi) = \langle f(t), \chi \rangle \quad \text{for } t > 0 \text{ and } \chi \in \dot{H}^1, \tag{5.2}$$

with $u(0) = u_0$. Now we proceed to a spatially discrete scheme based on the time discretization scheme given by (2.7), in which, for $n \geqslant 1$, we have that $U_h^n \in V_h$ satisfies

$$\langle U_h^n - U_h^{n-1}, \chi \rangle + \int_{t_{n-1}}^{t_n} \mathsf{A}(\mathfrak{D}_\alpha(\overline{U}_h)(t), \chi) \mathrm{d}s = \langle \tilde{f}^n, \chi \rangle \quad \text{for all } \chi \in V_h \tag{5.3}$$

with suitable approximations $U_h^0 \approx u_0$.

We define a finite-dimensional linear operator $A_h \colon V_h \to V_h$ by

$$\langle A_h v, \chi \rangle = \mathsf{A}(v, \chi) \quad \text{for all } v, \chi \in V_h,$$

and let $P_h \colon L_2(\Omega) \to V_h$ denote the orthoprojector, so that $\langle P_h v, \chi \rangle = \langle v, \chi \rangle$ for all $v \in L_2(\Omega)$ and $\chi \in V_h$. The problem (5.3) is equivalent to

$$U_h^n - U_h^{n-1} + \int_{t_{n-1}}^{t_n} \mathfrak{D}_\alpha(A_h \overline{U}_h)(t) \mathrm{d}t = P_h \tilde{f}^n \quad \text{for } n \geqslant 1.$$

Since the finite-dimensional operator $A_h \colon V_h \to V_h$ satisfies all of the properties required of $A \colon \dot{H}^1 \to \dot{H}^1$, the stability of (2.7) follows from Theorem 3.1, i.e.,

$$\|U_h^n\| \leqslant \|U_h^0\| + 2 \sum_{j=1}^{n} \|P_h \tilde{f}^j\| \leqslant \|U_h^0\| + 2 \sum_{j=1}^{n} \|\tilde{f}^j\| \quad \text{for } n \geqslant 1. \tag{5.4}$$

THEOREM 5.1. Let u be the solution of the initial-value problem (2.2) and let $U_h^n \in V_h$ be the solution of the fully discrete scheme (5.3). Assume, in addition to the regularity property (2.5) with $0 < \sigma < 1$, that

$$\|u_0\|_{\dot{H}^2} + \|u(t_1)\|_{\dot{H}^2} \leqslant M \quad \text{and} \quad t\|u'(t)\|_{\dot{H}^2} \leqslant M \quad \text{for } 0 < t \leqslant T.$$

Then the error bound of Theorem 4.3 remains valid if, on the left-hand side, we replace U^n with U_h^n and, on the right-hand side, we remove $\|U^0 - u_0\|$ and insert the terms

$$\|U_h^0 - R_h u_0\| + Ch^2 \max(1, \log k^{-1}). \tag{5.5}$$

Proof. We divide the error into two terms as follows:

$$U_h^n - u(t_n) = \theta^n + \rho(t_n),$$

where

$$\theta^n = U_h^n - R_h u(t_n) \in V_h \quad \text{and} \quad \rho(t) = R_h u(t) - u(t).$$

Since the bound of the second term can be easily obtained, our main task is to estimate the first term θ^n. Let $\chi \in V_h$. Integrating (5.2) from $t = t_{n-1}$ to $t = t_n$, we get

$$\langle u(t_n) - u(t_{n-1}), \chi\rangle + \int_{t_{n-1}}^{t_n} \mathsf{A}(\mathfrak{D}_\alpha u(t), \chi)\mathrm{d}t = \langle \tilde{f}^n, \chi\rangle,$$

and hence, by comparing it with (5.3) and noting that

$$(U_h^n - U_h^{n-1}) - (u(t_n) - u(t_{n-1})) = (\theta^n - \theta^{n-1}) + (\rho(t_n) - \rho(t_{n-1}))$$

and, from the definition of the Ritz projector, that

$$\mathsf{A}(\bar{U}_h(s), \chi) - \mathsf{A}(u(s), \chi) = \mathsf{A}(\bar{\theta}(s), \chi) + \mathsf{A}(\bar{u}(s) - u(s), \chi) - \langle \bar{\rho}(s), \chi\rangle,$$

we get

$$\langle \theta^n - \theta^{n-1}, \chi\rangle + \int_{t_{n-1}}^{t_n} \mathsf{A}(\mathfrak{D}_\alpha \bar{\theta}(t), \chi)\mathrm{d}t = \langle \widehat{\eta}^{n-1/2}, \chi\rangle,$$

where $\widehat{\eta}^{n-1/2} = \eta^{n-1/2} + \widehat{\eta}_1^{n-1/2} + \widehat{\eta}_2^{n-1/2}$, for the same $\eta^{n-1/2}$ as in (4.2) and for

$$\widehat{\eta}_1^{n-1/2} = \int_{t_{n-1}}^{t_n} \mathfrak{D}_\alpha \bar{\rho}(t)\mathrm{d}t \quad \text{and} \quad \widehat{\eta}_2^{n-1/2} = \rho(t_{n-1}) - \rho(t_n).$$

Hence, applying the stability result (5.4) and noting that $\theta^0 = U_h^0 - R_h u_0$, we get

$$\|\theta^n\| \leqslant \|U_h^0 - R_h u_0\| + 2\sum_{j=1}^{n} \|\widehat{\eta}^{j-1/2}\| \quad \text{for } 1 \leqslant n \leqslant N.$$

Because $\eta^{n-1/2}$ was already dealt with in Theorem 4.3, it suffices to estimate $\widehat{\eta}_1^{j-1/2}$ and $\widehat{\eta}_2^{j-1/2}$. For the contribution from the $\widehat{\eta}_1^{j-1/2}$, integrating gives

$$\widehat{\eta}_1^{j-1/2} = \mathfrak{D}_{\alpha+1}\bar{\rho}(t_j) - \mathfrak{D}_{\alpha+1}\bar{\rho}(t_{j-1}) = \int_0^{t_j} \omega_{\alpha+1}(t_j - s)\bar{\rho}(s)\mathrm{d}s - \int_0^{t_{j-1}} \omega_{\alpha+1}(t_{j-1} - s)\bar{\rho}(s)\mathrm{d}s.$$

So, for $j = 1$ we have

$$\|\widehat{\eta}_1^{1/2}\| \leqslant \int_0^{t_1} \omega_{\alpha+1}(t_1 - s)\|\bar{\rho}(s)\|\mathrm{d}s = \|\rho(t_1)\|\omega_{\alpha+2}(k_1). \tag{5.6}$$

For $j \geqslant 2$ we split the first term of $\widehat{\eta}_1^{j-1/2}$ as follows:

$$\int_0^{t_j} \omega_{\alpha+1}(t_j - s)\bar{\rho}(s)\mathrm{d}s = \rho(t_1)\int_0^{t_1} \omega_{\alpha+1}(t_j - s)\mathrm{d}s + \frac{1}{2}\sum_{i=2}^{j}[\rho(t_i) + \rho(t_{i-1})] \times \int_{t_{i-1}}^{t_i} \omega_{\alpha+1}(t_j - s)\mathrm{d}s$$

$$= \rho(t_1)\int_0^{t_1}\omega_{\alpha+1}(t_j-s)\mathrm{d}s + \frac{1}{2}\sum_{i=2}^{j-1}[\rho(t_{i-1})-\rho(t_{i+1})]$$
$$\times\int_{t_1}^{t_i}\omega_{\alpha+1}(t_j-s)\mathrm{d}s$$
$$+\frac{1}{2}[\rho(t_j)+\rho(t_{j-1})]\int_{t_1}^{t_j}\omega_{\alpha+1}(t_j-s)\mathrm{d}s.$$

Similarly, splitting the second term of $\widehat{\eta}_1^{j-1/2}$, we obtain

$$\int_0^{t_{j-1}}\omega_{\alpha+1}(t_{j-1}-s)\bar{\rho}(s)\mathrm{d}s = \rho(t_1)\int_0^{t_1}\omega_{\alpha+1}(t_{j-1}-s)\mathrm{d}s$$
$$+\frac{1}{2}\sum_{i=2}^{j-2}[\rho(t_{i-1})-\rho(t_{i+1})]\int_{t_1}^{t_i}\omega_{\alpha+1}(t_{j-1}-s)\mathrm{d}s$$
$$+\frac{1}{2}[\rho(t_{j-1})+\rho(t_{j-2})]\int_{t_1}^{t_{j-1}}\omega_{\alpha+1}(t_{j-1}-s)\mathrm{d}s$$
$$=\rho(t_1)\int_0^{t_1}\omega_{\alpha+1}(t_{j-1}-s)\mathrm{d}s$$
$$+\frac{1}{2}\sum_{i=2}^{j-1}[\rho(t_{i-1})-\rho(t_{i+1})]\int_{t_1}^{t_i}\omega_{\alpha+1}(t_{j-1}-s)\mathrm{d}s$$
$$+\frac{1}{2}[\rho(t_j)+\rho(t_{j-1})]\int_{t_1}^{t_{j-1}}\omega_{\alpha+1}(t_{j-1}-s)\mathrm{d}s.$$

Hence we have

$$2\|\widehat{\eta}_1^{j-1/2}\| \leqslant 2\|\rho(t_1)\|\int_0^{t_1}|\omega_{\alpha+1}(t_{j-1}-s)-\omega_{\alpha+1}(t_j-s)|\mathrm{d}s$$
$$+\sum_{i=2}^{j-1}\|\rho(t_{i-1})-\rho(t_{i+1})\|\int_{t_1}^{t_i}|\omega_{\alpha+1}(t_{j-1}-s)-\omega_{\alpha+1}(t_j-s)|\mathrm{d}s$$
$$+\|\rho(t_j)+\rho(t_{j-1})\|\left|\int_{t_1}^{t_j}\omega_{\alpha+1}(t_j-s)\mathrm{d}s-\int_{t_1}^{t_{j-1}}\omega_{\alpha+1}(t_{j-1}-s)\mathrm{d}s\right|.$$

Since

$$\omega_{\alpha+1}(t_{j-1}-s)-\omega_{\alpha+1}(t_j-s) > 0$$

and

$$\int_{t_1}^{t_j}\omega_{\alpha+1}(t_j-s)\mathrm{d}s-\int_{t_1}^{t_{j-1}}\omega_{\alpha+1}(t_{j-1}-s)\mathrm{d}s=\omega_{\alpha+2}(t_j-t_1)-\omega_{\alpha+2}(t_{j-1}-t_1) > 0,$$

a change in the order of summation implies that

$$
\begin{aligned}
2\sum_{j=2}^{n}\|\widehat{\eta}_1^{j-1/2}\| \leqslant 2\|\rho(t_1)\|\int_0^{t_1}\sum_{j=2}^{n}[\omega_{\alpha+1}(t_{j-1}-s)-\omega_{\alpha+1}(t_j-s)]\mathrm{d}s \\
+\sum_{i=2}^{n-1}\|\rho(t_{i-1})-\rho(t_{i+1})\|\int_{t_1}^{t_i}\sum_{j=i+1}^{n}[\omega_{\alpha+1}(t_{j-1}-s)-\omega_{\alpha+1}(t_j-s)]\mathrm{d}s \\
+\max_{2\leqslant j\leqslant n}(\|\rho(t_j)+\rho(t_{j-1})\|)\sum_{j=2}^{n}[\omega_{\alpha+2}(t_j-t_1)-\omega_{\alpha+2}(t_{j-1}-t_1)] \\
\leqslant 2\|\rho(t_1)\|\int_0^{t_1}\omega_{\alpha+1}(t_1-s)\mathrm{d}s \\
+\sum_{i=2}^{n-1}\|\rho(t_{i+1})-\rho(t_{i-1})\|\int_{t_1}^{t_i}\omega_{\alpha+1}(t_i-s)\mathrm{d}s \\
+\max_{2\leqslant i\leqslant n}(\|\rho(t_i)+\rho(t_{i-1})\|)\,\omega_{\alpha+2}(t_n-t_1),
\end{aligned}
$$

and thus

$$
\begin{aligned}
2\sum_{j=2}^{n}\|\widehat{\eta}_1^{j-1/2}\| \leqslant 2\omega_{\alpha+2}(t_1)\|\rho(t_1)\| \\
+\omega_{\alpha+2}(t_n)\left(\sum_{i=2}^{n}\|\rho(t_i)-\rho(t_{i-1})\|+\max_{2\leqslant i\leqslant n}\|\rho(t_i)+\rho(t_{i-1})\|\right).
\end{aligned} \tag{5.7}
$$

For $i \geqslant 2$ we have

$$
\rho(t_i)-\rho(t_{i-1})=(R_h-I)[u(t_i)-u(t_{i-1})]=\int_{t_{i-1}}^{t_i}(R_h-I)u'(s)\mathrm{d}s,
$$

and so, using (5.1), with $u'(s)$ in place of υ, yields

$$
\sum_{i=2}^{n}\|\rho(t_i)-\rho(t_{i-1})\| \leqslant Ch^2\int_{t_1}^{t_n}\|u'(s)\|_{\dot{H}^2}\,\mathrm{d}s. \tag{5.8}
$$

For $1 \leqslant i \leqslant n$, from (5.1), with $u(t_i)$ in place of υ, we obtain

$$
\begin{aligned}
\|\rho(t_i)\| \leqslant Ch^2\|u(t_i)\|_{\dot{H}^2} \leqslant Ch^2\left(\|u(t_1)\|_{\dot{H}^2}+\int_{t_1}^{t_i}\|u'(s)\|_{\dot{H}^2}\,\mathrm{d}s\right) \\
\leqslant Ch^2\left(\|u(t_1)\|_{\dot{H}^2}+\int_{t_1}^{t_n}\|u'(s)\|_{\dot{H}^2}\,\mathrm{d}s\right),
\end{aligned}
$$

and hence

$$\|\rho(t_1)\| + \max_{2\leqslant i\leqslant n} \|\rho(t_i) + \rho(t_{i-1})\| \leqslant Ch^2 \left(\|u(t_1)\|_{\dot{H}^2} + \int_{t_1}^{t_n} \|u'(s)\|_{\dot{H}^2}\, \mathrm{d}s \right).$$

Using this and (5.8) in equations (5.6) and (5.7), we find that

$$\sum_{j=1}^{n} \|\widehat{\eta}_1^{j-1/2}\| \leqslant Ch^2 \left(\int_{t_1}^{t_n} \|u'(s)\|_{\dot{H}^2}\, \mathrm{d}s + \|u(t_1)\|_{\dot{H}^2} \right). \tag{5.9}$$

The bound of $\widehat{\eta}_2^{j-1/2}$ can be directly obtained from (5.8) and

$$\|\rho(t_1) - \rho(t_0)\| \leqslant Ch^2 \left(\|u(t_1)\|_{\dot{H}^2} + \|u_0\|_{\dot{H}^2} \right).$$

So we have

$$\sum_{j=1}^{n} \|\widehat{\eta}_2^{j-1/2}\| \leqslant Ch^2 \left(\int_{t_1}^{t_n} \|u'(s)\|_{\dot{H}^2}\, \mathrm{d}s + \|u(t_1)\|_{\dot{H}^2} + \|u_0\|_{\dot{H}^2} \right). \tag{5.10}$$

Finally, combining (5.9) and (5.10) and using the given regularity assumptions, we obtain the error bound (5.5). □

6. Numerical experiments

In this section the time-stepping scheme (2.7) and the fully discrete scheme (5.3) are applied to some problems of the form (2.2) with $\alpha = -0.5$. In each case the time interval is $[0, T] = [0, 1]$ and we employ a time mesh of the form (2.10) for various choices of the mesh grading parameter $\gamma \geqslant 1$.

6.1 *A purely time-dependent problem*

We consider

$$\frac{\mathrm{d}u}{\mathrm{d}t} + \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t \omega_{\alpha+1}(t-s)u(s)\mathrm{d}s = f(t) \quad \text{for } 0 < t < T \text{ with } u(0) = u_0. \tag{6.1}$$

Using the Mittag–Leffler function $E_\mu(x) = \sum_{p=0}^{\infty} x^p / \Gamma(1 + p\mu)$, we may write the exact solution as

$$u(t) = E_{\alpha+1}(-t^{\alpha+1})u_0 + \int_0^t E_{\alpha+1}(-s^{\alpha+1}) f(t-s)\mathrm{d}s.$$

Choosing the initial datum $u_0 = 1$ and a source term $f(t) = (\alpha + 2)t^{\alpha+1}$, we find that

$$u(t) = E_{\alpha+1}\left(-t^{\alpha+1}\right) + t\Gamma(\alpha+3)\left(1 - E_{\alpha+1,2}\left(-t^{\alpha+1}\right)\right). \tag{6.2}$$

Since the exact solution (6.2) behaves like $t^{\alpha+1}$ as $t \to 0^+$, we see that the regularity condition (2.5) holds for $\sigma = 2 + 2\alpha = 1$ and hence $(2 + \alpha)/\sigma = 1.5$. Thus, by Theorem 4.3, we expect $\mathcal{O}(k^\gamma)$ convergence if $1 \leqslant \gamma < 1.5$ and $\mathcal{O}(k^{1.5})$ convergence if $\gamma > 1.5$. The numerical results shown in Table 1 are consistent with these expectations.

TABLE 1 *The error* $\max_{0\leqslant n\leqslant N}|U^n - u(t_n)|$ *for the purely time-dependent problem* (6.1) *with different mesh gradings*

N	$\gamma = 1$		$\gamma = 2$		$\gamma = 3$	
40	4.48×10^{-3}		9.20×10^{-4}		8.22×10^{-4}	
80	2.55×10^{-3}	0.81	3.47×10^{-4}	1.40	3.06×10^{-4}	1.42
160	1.39×10^{-3}	0.87	1.28×10^{-4}	1.44	1.12×10^{-4}	1.45
320	7.40×10^{-4}	0.91	4.62×10^{-5}	1.47	4.07×10^{-5}	1.46
640	3.86×10^{-4}	0.94	1.65×10^{-5}	1.48	1.46×10^{-5}	1.47
1280	1.99×10^{-4}	0.96	5.99×10^{-6}	1.49	5.24×10^{-6}	1.48
Theory		1.00		1.50		1.50

TABLE 2 *The error* $\max_{0\leqslant n\leqslant N}\|U^n - u(t_n)\|_{L_2(\Omega)}$ *with different mesh gradings for a problem in one space dimension*

N	$\gamma = 1$		$\gamma = 1.5$		$\gamma = 2$	
81	9.33×10^{-3}		1.63×10^{-3}		5.42×10^{-4}	
256	3.89×10^{-3}	0.76	3.50×10^{-4}	1.34	9.64×10^{-5}	1.50
625	1.87×10^{-3}	0.82	9.91×10^{-5}	1.41	2.53×10^{-5}	1.50
1296	9.96×10^{-4}	0.86	3.44×10^{-5}	1.45	8.46×10^{-6}	1.50
Theory		1.00		1.50		1.50

6.2 *A problem in one space dimension*

Let $\Omega = (0, 1)$ and $Au = -u_{xx}$ and assume that $u = u(x, t)$ satisfies homogeneous Dirichlet boundary conditions $u(0, t) = 0 = u(1, t)$ for all $t \in [0, T] = [0, 1]$.

We choose the initial datum $u_0(x)$ and source term $f(x, t)$ such that the exact solution is

$$u(t, x) = \left(t^{\alpha+1} - \frac{\Gamma(\alpha + 2)}{\pi^2}\right)\sin(\pi x).$$

Once again, the regularity condition (2.5) holds for $\sigma = 2 + 2\alpha = 1$ and hence $(2 + \alpha)/\sigma = 1.5$.

We apply the scheme of Theorem 5.1 for t_n of the form (2.10) and with a uniform spatial mesh having $N^{3/4}$ subintervals, each of length $h = 1/N^{3/4} = k^{3/4}$, so that $h^2 = k^{1.5}$ and the convergence rate is determined by time discretization (ignoring a possible logarithmic factor). For our discrete initial datum U^0, we take the L_2 projection of u_0 onto the continuous piecewise-linear FE space S_h. The numerical results, shown in Table 2, are as expected in Theorems 4.3 and 5.1.

Acknowledgement

The support of the King Fahd University of Petroleum and Minerals is gratefully acknowledged.

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Appendix A

The next two technical lemmas helped us to relatively control the difficulty that appeared in bounding the error from the time discretization in Section 4.

LEMMA A.1 For $2 \leqslant i < j$ we have

$$k_i^3 \mathbf{K}_\alpha^{i-1,j-1} \geqslant k_{i-1}^3 \mathbf{K}_\alpha^{i,j}.$$

Proof. Recall that

$$\mathbf{K}_\alpha^{i-1,j-1} = \frac{-\alpha}{2\Gamma(\alpha+1)} \int_{t_{i-2}}^{t_{i-1}} (s - t_{i-2})(t_{i-1} - s)(t_{j-1} - s)^{\alpha-1}\, \mathrm{d}s.$$

Now we employ the substitution

$$s = \frac{(t_i - q)t_{i-2} + (q - t_{i-1})t_{i-1}}{k_i}$$

and get

$$\mathbf{K}_\alpha^{i-1,j-1} = \frac{-\alpha}{2\Gamma(\alpha+1)} \frac{k_{i-1}^3}{k_i^3} \int_{t_{i-1}}^{t_i} (q - t_{i-1})(t_i - q)(t_{j-1} - s)^{\alpha-1}\, \mathrm{d}q. \tag{A.1}$$

Since

$$\begin{aligned} q - s &= k_i^{-1}(k_i q - (t_i - q)t_{i-2} - (q - t_{i-1})t_{i-1}) = k_i^{-1}((k_i - k_{i-1})q - t_i t_{i-2} + t_{i-1}t_{i-1}) \\ &\leqslant k_i^{-1}((k_i - k_{i-1})t_i - t_i t_{i-2} + t_{i-1}t_{i-1}) = k_i \leqslant k_j, \end{aligned}$$

we have $t_{j-1} - s = t_j - q - k_j + q - s \leqslant t_j - q$, and thus $(t_{j-1} - s)^{\alpha-1} \geqslant (t_j - q)^{\alpha-1}$ for $i < j$ $(-1 < \alpha < 0)$. Using this in (A.1), we observe that

$$\mathbf{K}_\alpha^{i-1,j-1} \geqslant \frac{-\alpha}{2\Gamma(\alpha+1)} \frac{k_{i-1}^3}{k_i^3} \int_{t_{i-1}}^{t_i} (q - t_{i-1})(t_i - q)(t_j - q)^{\alpha-1}\, \mathrm{d}q = \frac{k_{i-1}^3}{k_i^3} \mathbf{K}_\alpha^{i,j}$$

and therefore the proof is complete. □

LEMMA A.2 For $1 \leqslant i < j \leqslant n$ with $n \leqslant N$ we have

$$\sum_{j=i+1}^{n} \mathbf{K}_\alpha^{i,j} \leqslant \frac{k_i}{2} \omega_{\alpha+2}(k_i).$$

Proof. Using (4.8) and integrating, we get

$$\begin{aligned} \mathbf{K}_\alpha^{i,j} &= \int_{t_{i-1}}^{t_i} (s - t_{i-1/2})\omega_{\alpha+1}(t_j - s)\mathrm{d}s \leqslant \frac{k_i}{2} \int_{t_{i-1}}^{t_i} \omega_{\alpha+1}(t_j - s)\mathrm{d}s \\ &= \frac{k_i}{2}[\omega_{\alpha+2}(t_j - t_{i-1}) - \omega_{\alpha+2}(t_j - t_i)]. \end{aligned}$$

Since $t_j - t_i = t_{j-1} - t_{i-1} + (k_j - k_i) \geqslant t_{j-1} - t_{i-1}$ for $i < j$, we have $\omega_{\alpha+2}(t_j - t_i) \geqslant \omega_{\alpha+2}(t_{j-1} - t_{i-1})$, and thus

$$\sum_{j=i+1}^{n} \mathbf{K}_\alpha^{i,j} \leqslant \frac{k_i}{2} \sum_{j=i+1}^{n} [\omega_{\alpha+2}(t_j - t_{i-1}) - \omega_{\alpha+2}(t_{j-1} - t_{i-1})] \leqslant \frac{k_i}{2} \omega_{\alpha+2}(k_i).$$ □