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A second-order accurate numerical method for a fractional wave equation

William McLean · Kassem Mustapha

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Abstract We study a generalized Crank–Nicolson scheme for the time discretization of a fractional wave equation, in combination with a space discretization by linear finite elements. The scheme uses a non-uniform grid in time to compensate for the singular behaviour of the exact solution at $t = 0$. With appropriate assumptions on the data and assuming that the spatial domain is convex or smooth, we show that the error is of order $k^2 + h^2$, where k and h are the parameters for the time and space meshes, respectively.

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1 Introduction

A variety of physical models [17] lead to partial integro-differential equations involving the Riemann–Liouville fractional integration operator of order $\alpha > 0$,

$$\mathscr{I}_\alpha v(t) = \int_0^t \beta(t-s)v(s)\,\mathrm{d}s \quad \text{where} \quad \beta(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)}. \tag{1.1}$$

W. McLean (✉)
School of Mathematics and Statistics, The University of New South Wales,
Sydney 2052, Australia
e-mail: w.mclean@unsw.edu.au

K. Mustapha
Department of Mathematical Sciences, KFUPM, Dhahran, 31261, Saudi Arabia
e-mail: kassem@kfupm.edu.sa

(Here, Γ denotes the usual gamma function.) For $0 < \alpha < 1$, we shall consider an initial value problem of the form [5,22]

$$\frac{\partial u}{\partial t} + \mathscr{I}_\alpha A u = f(t) \quad \text{for } t > 0, \text{ with } u(0) = u_0, \tag{1.2}$$

in which 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 data 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 $0 \le \lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots$. When $\mathbb{H}$ is infinite-dimensional we also require

$$\lambda_m \to \infty \quad \text{as} \quad m \to \infty. \tag{1.3}$$

In our standard example, sometimes described as a fractional wave equation [21], we take $\mathbb{H} = L_2(\Omega)$ for a bounded, Lipschitz domain $\Omega \subseteq \mathbb{R}^d$ and $A = -\nabla^2$ subject to homogeneous Dirichlet or Neumann boundary conditions. In this case, $u = u(x,t), f = f(x,t)$ and $u_0 = u_0(x)$ for $x \in \Omega$ and $t > 0$. We may also impose periodic boundary conditions when $\Omega = (0,1)^d$.

Our purpose in this paper is to revisit the analysis of one of a group of numerical methods introduced in earlier work by the first author and others [16]. The analysis in that paper treats only the discretization in time and yields a suboptimal error bound when applied to (1.2). Here we address also the discretization in space by finite elements and present numerical evidence that our improved error bounds are sharp (except perhaps for a logarithmic factor). In addition, we establish improved regularity estimates for the inhomogeneous equation with zero initial data that permit more realistic assumptions on $f(t)$. We remark that in [16] the operator A is assumed to be strictly positive-definite, which rules out, e.g., periodic or homogeneous Neumann boundary conditions if $A = -\nabla^2$.

For our numerical method, we introduce time levels $0 = t_0 < t_1 < t_2 < \cdots$ and put $k_n = t_n - t_{n-1}$ and $t_{n-1/2} = \frac{1}{2}(t_{n-1} + t_n)$ for $n \ge 1$. Given a grid function V^n we write $V^{n-1/2} = \frac{1}{2}(V^{n-1} + V^n)$ and define a piecewise-constant approximation

$$\bar{V}(t) = \begin{cases} V^1 & \text{for } t_0 < t < t_1, \\ V^{n-1/2} & \text{for } t_{n-1} < t < t_n \quad \text{and} \quad n \ge 2. \end{cases} \tag{1.4}$$

The modification on the first subinterval ensures that $\bar{V}$ does not depend on V^0, which is necessary for our numerical scheme in cases when u_0 is not sufficiently regular to belong to the domain of A. Using $\bar{V}$, we define a discrete fractional integral

$$\mathscr{I}_\alpha^{n-1/2} V = \frac{1}{k_n} \int_{t_{n-1}}^{t_n} \int_0^t \beta(t-s) \bar{V}(s)\, \mathrm{d}s\, \mathrm{d}t = \omega_{n1} V^1\, k_1 + \sum_{j=2}^{n} \omega_{nj} V^{j-1/2}\, k_j,$$

where

$$\omega_{nj} = \frac{1}{k_n\,k_j} \int\limits_{t_{n-1}}^{t_n} \int\limits_{t_{j-1}}^{\min(t,t_j)} \beta(t-s)\,\mathrm{d}s\,\mathrm{d}t > 0.$$

An alternative approach would be to employ convolution quadrature [10,11], but we do not want to be restricted to using uniform time steps. The somewhat unusual quadrature approximation $\mathscr{I}_\alpha^{n-1/2}V \approx \mathscr{I}_\alpha v(t_{n-1/2})$ is a kind of averaged, product-integration rule and is designed so that

$$V^1 \mathscr{I}_\alpha^{1/2} V\,k_1 + \sum_{j=2}^{n} V^{j-1/2} \mathscr{I}_\alpha^{j-1/2} V\,k_j = \int\limits_0^{t_n} \bar{V}(t) \int\limits_0^{t} \beta(t-s)\bar{V}(s)\,\mathrm{d}s\,\mathrm{d}t.$$

This identity ensures that the discrete quadratic form on the left is positive semi-definite, from which the stability of our numerical scheme follows by a simple energy argument. We also choose approximations

$$f^{n-1/2} \approx \frac{1}{k_n} \int\limits_{t_{n-1}}^{t_n} f(t)\,\mathrm{d}t \quad \text{for } n \geq 1, \tag{1.5}$$

that are assumed to satisfy

$$\left\| f^{1/2}\,k_1 - \int\limits_0^{t_1} f(t)\,\mathrm{d}t \right\| \leq C \int\limits_0^{t_1} t \|f'(t)\|\,\mathrm{d}t \tag{1.6}$$

and

$$\left\| f^{n-1/2}\,k_n - \int\limits_{t_{n-1}}^{t_n} f(t)\,\mathrm{d}t \right\| \leq Ck_n^2 \int\limits_{t_{n-1}}^{t_n} \|f''(t)\|\,\mathrm{d}t \quad \text{for } n \geq 2. \tag{1.7}$$

For example, $f^{n-1/2} = f(t_{n-1/2})$ or $f^{n-1/2} = \frac{1}{2}[f(t_{n-1}) + f(t_n)]$ are permissible, as one sees using the Peano kernel for the midpoint or trapezoidal rule.

Starting from an approximation $U^0 \approx u_0$ to the initial data, we consider a time discretization

$$\frac{U^n - U^{n-1}}{k_n} + \mathscr{I}_\alpha^{n-1/2} AU = f^{n-1/2} \quad \text{for } n \geq 1, \tag{1.8}$$

that generates an approximate solution $U^n \approx u(t_n)$. As in the classical Crank–Nicolson scheme for the heat equation, the backward difference formally approximates the time derivative $\partial u/\partial t$ to $O(k_n^2)$ at the midpoint $t_{n-1/2}$ of the nth subinterval. The scheme (1.8) is implicit because $\mathscr{I}_\alpha^{n-1/2}AU$ depends on U^n. Of course, unlike the case of the classical heat equation, at each step we must compute a sum involving the solution at *all* previous time levels.

Although (1.8) is formally second-order accurate, the error in U^n generally fails to be $O(k^2)$ if we use a uniform time step k, because the exact solution $u(t)$ is not sufficiently smooth near $t = 0$. We therefore employ a family of non-uniform meshes that concentrate the time levels near $t = 0$. These meshes are indexed by a positive parameter k, tending to zero, and we assume that for some fixed $\gamma \geq 1$,

$$k_n \leq C_\gamma k \min\bigl(1, t_n^{1-1/\gamma}\bigr) \quad \text{for } n \geq 1, \tag{1.9}$$

where the constant C_γ is independent of k. Since $k_1 = t_1$, this means in particular that the length of the first subinterval must be $O(k^\gamma)$, whereas for t_n bounded away from 0 we have $k_n = O(k)$. The larger the value of γ the stronger must be the concentration of time levels near $t = 0$. By contrast, for a family of uniform meshes our assumption (1.9) will hold only if $\gamma = 1$. In addition to (1.9), we assume that

$$t_1 = k_1 \geq c_\gamma k^\gamma \quad \text{and} \quad t_n \leq C_\gamma t_{n-1} \quad \text{for } n \geq 2. \tag{1.10}$$

Use of the mesh properties (1.9) and (1.10) is standard for integral equations in which the solution $u(s)$ possesses a fixed singularity at $s = 0$; see, e.g., [1,2,20]. In our case, the integrand $\beta(t-s)u(s)$ also possesses a moving singularity at $s = t$ that the quadrature approximation handles using product integration. It turns out that for our error analysis we require a further, and more restrictive, assumption on the time mesh,

$$0 \leq k_{n+1} - k_n \leq C_\gamma k^2 \min\bigl(1, t_n^{1-2/\gamma}\bigr) \quad \text{for } n \geq 2. \tag{1.11}$$

Thus, the step size must increase monotonically with no abrupt changes from one time level to the next. A typical example of a mesh satisfying all three assumptions (1.9), (1.10) and (1.11) for an interval $[0, T]$ is

$$t_n = (nk)^\gamma \quad \text{for } 0 \leq n \leq N \ \text{ with } \ k = \frac{T^{1/\gamma}}{N}. \tag{1.12}$$

If T were large, then in practice one would probably modify this mesh so that k_j is constant for $t_j \geq 1$, say; e.g., see [20].

The papers [14,16] study several time discretization methods for problems of the form

$$\frac{\partial u}{\partial t} + \int_0^t \beta(t-s)Au(s)\,\mathrm{d}s = f(t) \quad \text{for } t > 0, \ \text{with } \ u(0) = u_0, \tag{1.13}$$

in which the kernel β is assumed to be positive semi-definite:

$$\int_0^T v(t) \int_0^t \beta(t-s)v(s)\, \mathrm{d}s\, \mathrm{d}t \geq 0, \tag{1.14}$$

for all $T > 0$ and any continuous $v : [0, T] \to \mathbb{R}$. The weakly singular kernel in (1.1) has this property, as do many smooth kernels, e.g., $\beta(t) = e^{-at}$ with $a > 0$. The analysis in [14] requires uniform time steps and shows, in the case of a certain two-level, backward-difference scheme, that the error is $O(k^2)$ when β is smooth, but that this accuracy is reduced to $O(k^{1+\alpha})$ for the weakly-singular kernel in (1.1). Numerical experiments in [14] confirm that this predicted loss of accuracy occurs in practice even in a very simple case when $u_0 = f(t) = \phi_m$ is an eigenfunction of A. The subsequent paper [16] analyses a variety of schemes with non-uniform meshes. In particular, an error bound of order $O(k^{1+\alpha})$ is shown for our scheme (1.8) and a mesh of the type (1.12) with $\gamma > 2$. However, as we prove in Corollary 3.4, this error bound is not sharp: the error is $O(k^2)$ under reasonable assumptions on the regularity of the data u_0 and $f(t)$.

Many authors have considered numerical methods for problems of the form (1.13). Typically, the time discretization is effected by a combination of finite differences and quadratures. An early paper of Sanz-Serna [22] proved $O(k)$ convergence for such a scheme using a uniform mesh. Lopez-Marcos [9] subsequently considered a fully-discrete scheme in one space dimension applying the usual second central difference approximation of $Au = -\partial^2 u/\partial x^2$ for a uniform step size h, showing $O(k|\log k|^{1/2} + h^2)$ convergence. (The latter result is actually for a modified version of our problem incorporating a nonlinear term $u\, \partial u/\partial x$.) For the space discretization, Fairweather et al. [4,19,24] considered orthogonal spline collocation and mixed finite element methods as alternatives to finite differences or regular finite element methods.

Achieving a second-order accurate scheme for (1.2) has proved to be surprisingly difficult. Lubich et al. [12] proved error estimates in the case of non-smooth data for several schemes employing a uniform step-size and convolution quadrature [10,11] in time, combined with linear finite elements in space. In particular, they prove an error bound of order $O(t_n^{-2}k^2 + t_n^{-1-\alpha}h^2)$ for a scheme based on a two-level backward difference approximation to $\partial u/\partial t$. Recent work of Cuesta et al. [3] shows that the error for a similar time discretization is $O(k^2)$, uniformly for $0 \leq t_n \leq T$, provided the data are sufficiently regular.

We also mention an alternative style of time discretization [7,8,15] that uses an N-point quadrature rule in an approximate Laplace inversion formula to achieve $O(e^{-cN/\log N})$ accuracy for t in a compact subinterval of $(0, \infty)$. Apart from its extraordinarily high accuracy, an attractive feature of this type of scheme is that the elliptic solves, one for each quadrature point on a contour in the complex plane, are independent and may be solved in parallel. However, a difficulty with such schemes is the need to compute an analytic continuation of the Laplace transform of the inhomogeneous term $f(t)$. Also, it is unclear whether this approach can be modified to handle non-linear versions of (1.2) effectively. Hence, the need to achieve higher-order accuracy with time-stepping schemes remains.

It is important to note that if the domain Ω is not convex or $C^{1,1}$, then in practice the exact solution will generally not possess sufficient regularity to achieve second-order accuracy for the space discretization. This loss of accuracy might be addressed by employing suitable local refinement of the finite element mesh, but such an approach is beyond the scope of the present work.

An outline of the paper is as follows. Section 2 discusses the regularity of the exact solution and serves to introduce some norms and other notation needed for our analysis. Section 3 proves the main result of the paper, Theorem 3.3, that gives our improved error bounds for the time discretization. In Sect. 4, we describe a spatially-discrete version of (1.8) employing linear finite elements, and show that the additional error is $O(h^2|\log k|)$, so that we achieve essentially second-order accuracy in space as well as in time. Finally, Sect. 5 presents some numerical studies of a few test problems.

2 Regularity of the exact solution

In this section, we seek to show that the solution of (1.2) satisfies

$$\|Au(t)\| + t\|Au'(t)\| + t^2\|Au''(t)\| = O(t^{\sigma-1}) \quad \text{as } t \to 0^+, \text{with } \sigma > 0. \tag{2.1}$$

This type of regularity result will allow us to bound the error arising from the time discretization. In addition, to eventually obtain a bound for the additional error due to the space discretization, we seek to show that, for the Sobolev norm $\|v\|_r$ defined below,

$$\|u(t)\|_r + t\|u'(t)\|_r = O(t^\nu) \quad \text{as } t \to 0^+, \text{with } 0 \le r \le 2 \text{ and } \nu \ge 0. \tag{2.2}$$

Our overall approach follows [14, Sect. 5], but with some modifications that yield improved results for the inhomogeneous equation.

Our bounds are expressed in terms of the norm

$$\|v\|_r^2 = \|(I+A)^{r/2}v\|^2 = \sum_{m=1}^{\infty}(1+\lambda_m)^r\langle v,\phi_m\rangle^2, \quad -\infty < r < \infty,$$

and the associated real Hilbert space $\dot{H}^r = \{v \in \mathbb{H} : \|v\|_r < \infty\}$. Obviously $\dot{H}^0 = \mathbb{H}$ and, in view of our assumptions (1.3) on the eigenvalues of A, we have $\dot{H}^r \subseteq \dot{H}^s$ for $s < r$. Also associated with the linear operator A is a bilinear form

$$\mathsf{A}(v,\chi) = \langle Av,\chi\rangle = \sum_{m=1}^{\infty}\lambda_m\langle v,\phi_m\rangle\langle\phi_m,\chi\rangle \quad \text{for } v, \chi \in \dot{H}^1. \tag{2.3}$$

The spaces $\dot{H}^r$ are commonly used in studying the regularity of parabolic problems [23, Chap. 3] so here we merely summarize their relevant properties without proof.

In our standard examples, when $A = -\nabla^2$ and $\mathbb{H} = L_2(\Omega)$, we find that $\dot{H}^r$ is a subspace of the Sobolev space $H^r(\Omega)$, depending on the boundary conditions incorporated in the definition of the eigenfunctions. Let us consider the three cases: homogeneous Dirichlet,

$$u(x,t) = 0 \quad \text{for } x \in \partial\Omega \quad \text{and} \quad t > 0; \tag{2.4}$$

homogeneous Neumann,

$$\partial_n u(x,t) = 0 \quad \text{for } x \in \partial\Omega \quad \text{and} \quad t > 0; \tag{2.5}$$

and unit-periodic,

$$u(x + e_j, t) = u(x,t) \quad \text{for } x \in \mathbb{R}^d, t > 0 \quad \text{and} \quad j = 1, 2, \ldots, d,$$

where e_j is the jth standard basis vector. We denote the Dirichlet, Neumann and periodic eigenfunctions by ϕ_m^{D}, ϕ_m^{N} and ϕ_m^{P}, respectively, so that $\phi_m^{\mathrm{D}} = \partial_n \phi_m^{\mathrm{N}} = 0$ on $\partial\Omega$ and $\phi_m^{\mathrm{P}}(x+e_j) = \phi_m^{\mathrm{P}}(x)$. These choices for ϕ_m yield corresponding Hilbert spaces $\dot{H}^r$ that we denote by $\dot{H}^r_{\mathrm{D}}$, $\dot{H}^r_{\mathrm{N}}$ and $\dot{H}^r_{\mathrm{P}}$, respectively. The periodic case is the simplest:

$$\dot{H}^r_{\mathrm{P}} = H^r(\mathbb{T}^d) \quad \text{for } -\infty < r < \infty,$$

where $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$ denotes the d-torus.

In all three cases, the first Green identity implies that the bilinear form (2.3) is given by

$$\mathsf{A}(v, \chi) = \int_\Omega \nabla v \cdot \nabla \chi \, \mathrm{d}x \quad \text{for } v, \chi \in \dot{H}^1,$$

and that $\mathsf{A}(v, \phi_m) = \lambda_m \langle v, \phi_m \rangle$. Our assumptions on Ω suffice to ensure that

$$\dot{H}^r_{\mathrm{D}} = \widetilde{H}^r(\Omega) \;\text{ and }\; \dot{H}^r_{\mathrm{N}} = H^r(\Omega) \quad \text{for } 0 < r \le 1.$$

If Ω is such that $\|v\|_{H^r(\Omega)} \le C\big(\|\nabla^2 v\|_{H^{r-2}(\Omega)} + \|v\|_{L_2(\Omega)}\big)$ holds for an integer $r \ge 2$, then

$$\begin{aligned}
\dot{H}^r_{\mathrm{D}} &= \{\, v \in H^r(\Omega) : \nabla^{2j} v = 0 \text{ on } \partial\Omega \text{ for all integers } j < r/2 \,\},\\
\dot{H}^r_{\mathrm{N}} &= \{\, v \in H^r(\Omega) : \partial_n \nabla^{2j} v = 0 \text{ on } \partial\Omega \text{ for all integers } j < (r-1)/2 \,\}.
\end{aligned}$$

In particular, if Ω is convex or $C^{1,1}$, then we may take $r = 2$.

A regularity theory for our initial value problem (1.2) may be developed from an eigenfunction expansion of the solution. Indeed, if we denote the Fourier coefficients of $u(t)$, $f(t)$ and u_0 by

$$u_m(t) = \langle u(t), \phi_m \rangle, \quad f_m(t) = \langle f(t), \phi_m \rangle, \quad u_{0m} = \langle u_0, \phi_m \rangle,$$

then we obtain the sequence of scalar initial value problems

$$\frac{\mathrm{d}u_m}{\mathrm{d}t} + \lambda_m \mathscr{I}_\alpha u_m = f_m(t) \quad \text{for } t > 0, \text{ with } u_m(0) = u_{0m}. \tag{2.6}$$

Denoting the Laplace transform of v by $\hat{v}(z) = \mathscr{L}\{v(t)\} = \int_0^\infty e^{-zt} v(t)\,\mathrm{d}t$, we have

$$\mathscr{L}\{t^{\mu-1}/\Gamma(\mu)\} = z^{-\mu} \quad \text{for } \mu > 0. \tag{2.7}$$

Hence, writing $*$ for the Laplace convolution,

$$\widehat{\mathscr{I}_\alpha v}(z) = \mathscr{L}\{\beta * v\} = \hat{\beta}(z)\hat{v}(z) \text{ and } \hat{\beta}(z) = z^{-\alpha}.$$

It follows that the Laplace transform of u_m is $\hat{u}_m(z) = (z + \lambda_m z^{-\alpha})^{-1}[u_{0m} + \hat{f}_m(z)]$. The Mittag–Leffler function [6,18], [17, Appendix B],

$$E_\mu(t) = \sum_{p=0}^{\infty} \frac{t^p}{\Gamma(1+\mu p)}, \tag{2.8}$$

arises when we compute the inverse Laplace transform

$$\mathscr{L}^{-1}\left\{(z + \lambda_m z^{-\alpha})^{-1}\right\} = \mathscr{L}^{-1}\left\{\sum_{p=0}^{\infty} (-\lambda_m)^p z^{-(1+\alpha)p-1}\right\} = E_{1+\alpha}(-\lambda_m t^{1+\alpha}).$$

We therefore define a linear operator

$$\mathscr{E}(t)v = \sum_{m=1}^{\infty} \langle v, \phi_m \rangle E_{1+\alpha}(-\lambda_m t^{1+\alpha})\phi_m, \tag{2.9}$$

so that $u(t) = \mathscr{E}(t)u_0$ is the solution of (1.2) when $f(t) \equiv 0$, and in general

$$u(t) = \mathscr{E}(t)u_0 + \int_0^t \mathscr{E}(t-s)f(s)\,\mathrm{d}s. \tag{2.10}$$

It can be shown that $|E_{1+\alpha}(-t)| \le 1$ for $t \ge 0$, so $\|\mathscr{E}(t)v\| \le \|v\|$ and the continuous problem is stable in $\mathbb{H}$:

$$\|u(t)\| \le \|u_0\| + \int_0^t \|f(s)\|\,\mathrm{d}s. \tag{2.11}$$

We now state a regularity result for the homogeneous problem.

Theorem 2.1 *Let* $0 < \alpha < 1$, $-\infty < r < \infty$ *and* $t > 0$. *The solution operator* (2.9) *for the homogeneous equation satisfies*

$$\|\mathscr{E}(t)v\|_{r+\mu} \le C_\alpha t^{-(1+\alpha)\mu/2}\|v\|_r \quad \textit{for } 0 \le \mu \le 2,$$

and for $q = 1, 2, 3, \ldots$,

$$t^q \left\|\mathscr{E}^{(q)}(t)v\right\|_{r+\mu} \le C_{\alpha,q} t^{-(1+\alpha)\mu/2}\|v\|_r \quad \textit{for } -2 \le \mu \le 2.$$

Proof See [14, Theorem 5.5]. □

As an immediate consequence we obtain bounds of the form (2.1) and (2.2) for the homogeneous problem.

Corollary 2.2 *Let* u *be the solution of* (1.2) *when* $f(t) \equiv 0$. *If*

$$\sigma = \frac{r}{2}(1+\alpha) - \alpha \quad \textit{and} \quad \nu = \frac{r-\kappa}{2}(1+\alpha)$$

then

$$\begin{aligned} \|Au(t)\| &\le C_\alpha t^{\sigma-1}\|u_0\|_r \quad \textit{for } 0 \le r \le 2, \\ t\|Au'(t)\| + t^2\|Au''(t)\| &\le C_\alpha t^{\sigma-1}\|u_0\|_r \quad \textit{for } 0 \le r \le 4, \end{aligned}$$

and

$$\begin{aligned} \|u(t)\|_\kappa &\le C_\alpha t^\nu \|u_0\|_r \qquad \textit{for } \kappa - 2 \le r \le \kappa, \\ t\|u'(t)\|_\kappa &\le C_\alpha t^\nu \|u_0\|_r \qquad \textit{for } \kappa - 2 \le r \le \kappa + 2. \end{aligned}$$

Proof For $0 \le 2 - r \le 2$, i.e., for $0 \le r \le 2$, we have

$$\|Au(t)\| \le \|u(t)\|_2 = \|u(t)\|_{r+(2-r)} \le C_\alpha t^{-(1+\alpha)(2-r)/2}\|u_0\|_r,$$

and $-(1+\alpha)(2-r)/2 = \sigma - 1$. The second estimate follows in a similar fashion for $-2 \le 2 - r \le 2$, i.e., for $0 \le r \le 4$.

Similarly, for $0 \le \kappa - r \le 2$, i.e., for $\kappa - 2 \le r \le \kappa$, we have

$$\|u(t)\|_r = \|u(t)\|_{r+(\kappa-r)} \le C_\alpha t^{-(1+\alpha)(\kappa-r)/2}\|u_0\|_r = C_\alpha t^\nu \|u_0\|_r,$$

and the final estimate holds for $-2 \le \kappa - r \le 2$, i.e., for $\kappa - 2 \le r \le \kappa + 2$. □

The next theorem concerns the inhomogeneous equation with zero initial data, and is an improved version of [14, Theorem 5.6]. In the proof, we go to some trouble to minimise the spatial regularity requirements on f, at the expense of demanding increased regularity in time, to avoid imposing artificial conditions on the boundary values of f. The proof relies on the following lemma.

Lemma 2.3 $\|v - \mathscr{E}(t)v\|_r \le C_\alpha t^{(1+\alpha)\mu/2}\|v\|_{r+\mu}$ *for* $0 \le \mu \le 2$.

Proof It can be shown [14, Lemma 5.2] that the Mittag–Leffler function satisfies

$$|E_{1+\alpha}(-t) - 1| \le C_\alpha \min(t, 1) \le C_\alpha t^{\mu/2} \quad \text{for } t > 0 \text{ and } 0 \le \mu \le 2,$$

so

$$\begin{aligned}\|v - \mathscr{E}(t)v\|_r^2 &= \sum_{m=1}^{\infty}(1+\lambda_m)^r\langle v, \phi_m\rangle^2\big|E_{1+\alpha}(-\lambda_m t^{1+\alpha}) - 1\big|^2 \\ &\le C_\alpha \sum_{m=1}^{\infty}(1+\lambda_m)^r\langle v, \phi_m\rangle^2(\lambda_m t^{1+\alpha})^\mu \\ &\le C_\alpha t^{(1+\alpha)\mu}\sum_{m=1}^{\infty}(1+\lambda_m)^{r+\mu}\langle v, \phi_m\rangle^2 = C_\alpha\big(t^{(1+\alpha)\mu/2}\|v\|_{r+\mu}\big)^2.\end{aligned}$$

□

Theorem 2.4 *Let* $0 < \alpha < 1$, $-\infty < r < \infty$ *and* $t > 0$*. If* $u_0 = 0$ *then for* $0 \le \mu \le 2$, $q = 0, 1, 2, \dots$ *and* $0 < t \le T$*, the solution of* (1.2) *satisfies*

$$t^q\|u^{(q)}(t)\|_{r+2} \le C_{\alpha,q,T}\left(t^{(1+\alpha)\mu/2-\alpha}\|f(0)\|_{r+\mu} + \sum_{j=0}^{q+1} t^{-\alpha}\int_0^t s^j\|f^{(j+1)}(s)\|_r\,ds\right).$$

Proof Let $\omega_\mu(t) = t^{\mu-1}/\Gamma(\mu)$ and recall from (2.7) that $\widehat{\omega}_\mu(z) = z^{-\mu}$. Thus,

$$\omega_\mu * \omega_\nu = \omega_{\mu+\nu} \quad \text{for } \mu > 0, \nu > 0, \tag{2.12}$$

and in particular, since $\beta = \omega_\alpha$, we have $\omega_{1-\alpha} * \beta = \omega_{1-\alpha} * \omega_\alpha = \omega_1 = 1$, which implies the Abel inversion formula:

$$\int_0^t v(s)\,\mathrm{d}s = (\omega_1 * v)(t) = \omega_{1-\alpha} * (\beta * v)(t).$$

Taking $v(t) = \lambda_m u_m(t)$ we see from (2.6) that $\beta * v = f_m - u'_m$ so

$$\omega_1 * Au = \sum_{m=1}^{\infty} \omega_1 * \lambda_m u_m \, \phi_m = \sum_{m=1}^{\infty} \omega_{1-\alpha} * (f_m - u'_m) \, \phi_m = \omega_{1-\alpha} * (f - u'), \quad (2.13)$$

or in other words

$$\int_0^t Au(s) \, \mathrm{d}s = \int_0^t \frac{(t-s)^{-\alpha}}{\Gamma(1-\alpha)} [f(s) - u'(s)] \, \mathrm{d}s.$$

Introducing the differential operator $(Dv)(t) = tv'(t)$, a short calculation shows

$$D(w * v) = w * v + (Dw) * v + w * (Dv). \quad (2.14)$$

In particular, since $D\omega_\mu = (\mu - 1)\omega_\mu$,

$$D(\omega_\mu * v) = \omega_\mu * (D + \mu)v, \quad (2.15)$$

and so by (2.13),

$$D(\omega_1 * Au) = \omega_{1-\alpha} * (D + 1 - \alpha)(f - u'). \quad (2.16)$$

From $D(\omega_1 * v)(t) = tv(t)$ we conclude that

$$tAu(t) = \int_0^t \frac{(t-s)^{-\alpha}}{\Gamma(1-\alpha)} \left(s \frac{\mathrm{d}}{\mathrm{d}s} + 1 - \alpha \right) [f(s) - u'(s)] \, \mathrm{d}s.$$

An induction on q shows that, for some constants a_{qj}, we have the identities

$$t^q v^{(q)}(t) = t^{-1} \sum_{j=0}^{q} a_{qj} D^j(tv) \quad \text{and} \quad D^q(tv) = t \sum_{j=0}^{q} \binom{q}{j} D^j v,$$

so to bound $t^q \|u^{(q)}(t)\|_{r+2}$ it suffices to consider

$$\begin{aligned} t^{-1}\|D^q(tu)\|_{r+2} &= t^{-1}\|(I + A)D^q(tu)\|_r \le t^{-1}\|D^q(tu)\|_r + t^{-1}\|D^q(tAu)\|_r \\ &\le C_q \sum_{j=0}^{q} \|D^j u\|_r + t^{-1}\|D^q(tAu)\|_r. \end{aligned}$$

Equations (2.15) and (2.16) give $D^q(tAu) = \omega_{1-\alpha} * \big[(D+1-\alpha)^{q+1}(f-u')\big]$, so

$$t^{-1}\|D^q(tu)\|_{r+2} \le C_q\left(\sum_{j=0}^{q}\|D^j u\|_r + t^{-1}\sum_{j=0}^{q+1}\omega_{1-\alpha} * \big\|D^j(f-u')\big\|_r\right). \tag{2.17}$$

The representation (2.10) with $u_0 = 0$ means that $u = \mathscr{E} * f$, and the identity (2.14) shows, for some constants b_{jlm}, that $D^j(w*v) = \sum_{l+m\le j} b_{jlm} D^l w * D^m v$. By Theorem 2.1, we have $\|(D^l\mathscr{E})(t)v\|_r \le C_{l,\alpha}\|v\|_r$, so

$$\|D^j u\|_r \le C_j \sum_{l+m\le j}\int_0^t \big\|D^l\mathscr{E}(t-s)D^m f(s)\big\|_r\,\mathrm{d}s \le C_{j,\alpha}\sum_{m=0}^{j}\int_0^t \|D^m f(s)\|_r\,\mathrm{d}s,$$

and since

$$\int_0^t \|f(s)\|_r\,\mathrm{d}s \le \int_0^t\left(\|f(0)\|_r + \int_0^s \|f'(\xi)\|_r\,d\xi\right)\mathrm{d}s$$
$$= t\|f(0)\|_r + \int_0^t (t-s)\|f'(s)\|_r\,\mathrm{d}s,$$

we obtain the bound

$$\sum_{j=0}^{q}\|D^j u\|_r \le C_{\alpha,q}t\left(\|f(0)\|_r + \sum_{j=0}^{q-1}\int_0^t s^j\|f^{(j+1)}(s)\|_r\,\mathrm{d}s\right). \tag{2.18}$$

To handle the remaining terms in (2.17), we write $u(t) = \int_0^t \mathscr{E}(s)f(t-s)\,\mathrm{d}s$ and then differentiate to obtain $u'(t) = \mathscr{E}(t)f(0) + \int_0^t \mathscr{E}(s)f'(t-s)\,\mathrm{d}s$. In this way,

$$f(t) - u'(t) = f(0) - \mathscr{E}(t)f(0) + \int_0^t \big[f'(s) - \mathscr{E}(s)f'(t-s)\big]\,\mathrm{d}s. \tag{2.19}$$

Using Theorem 2.1 and Lemma 2.3 we find that

$$\|f(t) - u'(t)\|_r \le \|f(0) - \mathscr{E}(t)f(0)\|_r + C_\alpha\int_0^t \|f'(s)\|_r\,\mathrm{d}s$$
$$\le C_\alpha t^{(1+\alpha)\mu/2}\|f(0)\|_{r+\mu} + C_\alpha(\omega_1 * \|f'\|_r),$$

and hence

$$
\begin{aligned}
t^{-1}\omega_{1-\alpha} \; * \|f-u'\|_r &\le C_\alpha t^{-1}\Big(\omega_{1-\alpha} * \omega_{(1+\alpha)\mu/2+1}\|f(0)\|_{r+\mu} + \omega_{2-\alpha} * \|f'\|_r\Big)\\
&\le C_\alpha t^{-1}\left(t^{(1+\alpha)\mu/2+1-\alpha}\|f(0)\|_{r+\mu} + \int_0^t \frac{(t-s)^{1-\alpha}}{\Gamma(2-\alpha)}\|f'(s)\|_r\,\mathrm{d}s\right)\\
&\le C_\alpha\left(t^{(1+\alpha)\mu/2-\alpha}\|f(0)\|_{r+\mu} + t^{-\alpha}\int_0^t \|f'(s)\|_r\,\mathrm{d}s\right).
\end{aligned}
$$

For $j \ge 1$, we have

$$
D^j(f-u') = -(D^j\mathscr{E})f(0) + \omega_1 * (D+1)^j f' - \sum_{l+m\le j} b_{jlm} D^l\mathscr{E} * D^m f'
$$

so, applying Theorem 2.1,

$$
\|D^j(f-u')\|_r \le C_{\alpha,j}\Big(t^{(1+\alpha)\mu/2}\|f(0)\|_{r+\mu} + \sum_{m=0}^{j}\int_0^t \|D^m f'(s)\|_r\,\mathrm{d}s\Big),
$$

and therefore

$$
\begin{aligned}
&t^{-1}\sum_{j=0}^{q+1}\omega_{1-\alpha} * \|D^j(f-u')\|_r\\
&\qquad\le C_{\alpha,q}\Big(t^{(1+\alpha)\mu/2-\alpha}\|f(0)\|_{r+\mu} + \sum_{j=0}^{q+1} t^{-\alpha}\int_0^t \|D^j f'(s)\|_r\,\mathrm{d}s\Big).
\end{aligned}
$$

Inserting this bound and (2.18) into (2.17) yields the conclusion of the theorem. □

Bounds of the form (2.1) and (2.2) now follow for the inhomogeneous problem with zero initial data.

Corollary 2.5 *Let u be the solution of* (1.2) *when $u_0 = 0$. If*

$$
\sigma = \frac{r}{2}(1+\alpha) + 1 - \alpha \quad \textit{and} \quad \nu = 1 + \frac{r-\kappa}{2}(1+\alpha) \quad \textit{with } 0 \le \kappa \le 2,
$$

then

$$
\begin{aligned}
\|Au(t)\| + t\|Au'(t)\| + t^2\|Au''(t)\| &\le C_\alpha t^{\sigma-1}\|f(0)\|_r\\
&\quad + C_\alpha t^{-\alpha}\sum_{j=1}^{3}\int_0^t s^j\|f^{(j+1)}(s)\|\,ds \quad \textit{for } 0 \le r \le 2
\end{aligned}
$$

and

$$\|u(t)\|_\kappa + t\|u'(t)\|_\kappa \le C_\alpha t^\nu \|f(0)\|_r + C_\alpha t^{-\alpha} \sum_{j=1}^{2} \int_0^t s^j \|f^{(j+1)}(s)\|\,\mathrm{d}s \quad \text{for } \kappa - 2 \le r \le \kappa.$$

Proof Theorem 2.4 implies that for $0 \le r \le 2$,

$$\|u(t)\|_2 + t\|u'(t)\|_2 + t^2\|u''(t)\|_2 = \|u(t)\|_{0+2} + t\|u'(t)\|_{0+2} + t^2\|u''(t)\|_{0+2} \le C_\alpha t^{(1+\alpha)r/2-\alpha}\|f(0)\|_{0+r} + C_\alpha t^{-\alpha} \sum_{j=0}^{3} \int_0^t s^j \|f^{(j+1)}(s)\|_0\,\mathrm{d}s.$$

which proves the first estimate. If $0 \le r + 2 - \kappa \le 2$, i.e., if $\kappa - 2 \le r \le \kappa$, then

$$\begin{aligned}\|u(t)\|_\kappa + t\|u'(t)\|_\kappa &= \|u(t)\|_{(\kappa-2)+2} + t\|u'(t)\|_{(\kappa-2)+2} \\ &\le C_\alpha t^{(1+\alpha)(r+2-\kappa)/2-\alpha}\|f(0)\|_{(\kappa-2)+(r+2-\kappa)} \\ &\quad + C_\alpha t^{-\alpha}\sum_{j=0}^{2}\int_0^t s^j \|f^{(j+1)}(s)\|_{\kappa-2}\,\mathrm{d}s,\end{aligned}$$

and the second estimate follows after noting that $(1+\alpha)(r+2-\kappa)/2 - \alpha = \nu$ and $\|f^{(j+1)}(s)\|_{\kappa-2} \le \|f^{(j+1)}(s)\|$ for $\kappa \le 2$. □

Remark 2.6 Corollaries 2.2 and 2.5 show that to have $\sigma > 0$ the initial data must satisfy $u_0 \in \dot{H}^r$ for some $r > 2\alpha/(1+\alpha)$, whereas no spatial regularity is needed for f. By comparison, to have $\nu \ge 0$ we require $u_0 \in \dot{H}^\kappa$ and $f(0) \in \dot{H}^{\kappa-2/(1+\alpha)}$. Therefore, to achieve second-order accuracy for the discrete-time, discrete-space scheme, we set $\kappa = 2$ and see that the spatial regularity requirements on the data are $u_0 \in \dot{H}^2$ and $f(0) \in \dot{H}^{2\alpha/(1+\alpha)}$.

Since $\dot{H}^r_{\mathrm{D}} = H^r(\Omega)$ only if $r < 1/2$, it follows that in the case of homogeneous Dirichlet boundary conditions (2.4) our error analysis will prove second-order accuracy with a suitable mesh grading and for sufficiently smooth data, provided $u_0 = 0$ on $\partial\Omega$ and, when $1/3 \le \alpha < 1$, $f(0) = 0$ on $\partial\Omega$. However, since $\dot{H}^1_{\mathrm{N}} = H^1(\Omega)$, with homogeneous Neumann boundary conditions (2.5) we have no restriction on the boundary values of $f(0)$, but require $\partial_n u_0 = 0$ on $\partial\Omega$.

3 Error from the time discretization

Our task in this section is to estimate the error $e^n = U^n - u(t_n)$ when U^n is given by (1.8). We begin by noting that the scheme is unconditionally stable.

Theorem 3.1 *For each U^0, $f^{1/2}$, $f^{3/2}, \dots, f^{n-1/2}$ in $\mathbb{H}$, the discrete initial-value problem* (1.8) *has a unique solution U^1, $U^2, \dots, U^n$ in $\mathbb{H}$. Furthermore,*

$$U^n \in \dot{H}^2 \quad \text{and} \quad \|U^n\| \le \|U^0\| + 2\sum_{j=1}^{n} \|f^{j-1/2}\|\, k_j \quad \text{for } n \ge 1.$$

Proof See [16, Lemma 4.1 and Theorem 7.1] or [13, Theorem 3.2]. □

The scheme (1.8) may be written as

$$U^n - U^{n-1} + \int_{t_{n-1}}^{t_n} \int_0^t \beta(t-s) A\bar{U}(s)\, \mathrm{d}s\, \mathrm{d}t = f^{n-1/2}\, k_n. \tag{3.1}$$

For comparison, integrating (1.2) from $t = t_{n-1}$ to $t = t_n$ shows that

$$u(t_n) - u(t_{n-1}) + \int_{t_{n-1}}^{t_n} \int_0^t \beta(t-s) Au(s)\, \mathrm{d}s\, \mathrm{d}t = \int_{t_{n-1}}^{t_n} f(t)\, \mathrm{d}t. \tag{3.2}$$

Hence, the error satisfies

$$e^n - e^{n-1} + \int_{t_{n-1}}^{t_n} \int_0^t \beta(t-s) A\bar{e}(s)\, \mathrm{d}s\, \mathrm{d}t = \eta^{n-1/2}\, k_n, \tag{3.3}$$

where $\eta^{n-1/2} = \eta_1^{n-1/2} + \eta_2^{n-1/2}$ with

$$\begin{aligned} \eta_1^{n-1/2} &= f^{n-1/2} - \frac{1}{k_n} \int_{t_{n-1}}^{t_n} f(t)\, \mathrm{d}t, \\ \eta_2^{n-1/2} &= \frac{1}{k_n} \int_{t_{n-1}}^{t_n} \int_0^t \beta(t-s) \big[Au(s) - A\bar{u}(s)\big]\, \mathrm{d}s\, \mathrm{d}t. \end{aligned} \tag{3.4}$$

Since (3.3) has the same form as (3.1), and since $e^0 = U^0 - u_0$, the stability result of Theorem 3.1 implies that

$$\|e^n\| \le \|U^0 - u_0\| + 2\sum_{j=1}^{n} \|\eta^{j-1/2}\|\, k_j \quad \text{for } n \ge 1. \tag{3.5}$$

Thus, our task reduces to estimating the sum on the right hand side of this inequality. The contribution from $\eta_1^{j-1/2}$ is easily controlled if one assumes (1.6) and (1.7), but $\eta_2^{j-1/2}$ gives much more trouble.

We introduce the continuous, piecewise-linear interpolant

$$\check{u}(t) = \begin{cases} u(t_1) & \text{for } 0 < t < t_1, \\ k_i^{-1}\big[(t_i - t)u(t_{i-1}) + (t - t_{i-1})u(t_i)\big] & \text{for } t_{i-1} \le t \le t_i \text{ and } i \ge 2, \end{cases}$$

and make the splitting $\eta_2^{j-1/2} = \eta_{21}^{j-1/2} + \eta_{22}^{j-1/2}$, where

$$\begin{aligned} \eta_{21}^{j-1/2} &= \frac{1}{k_j}\int_{t_{j-1}}^{t_j}\int_0^t \beta(t-s)\big[Au(s) - A\check{u}(s)\big]\,\mathrm{d}s\,\mathrm{d}t, \\ \eta_{22}^{j-1/2} &= \frac{1}{k_j}\int_{t_{j-1}}^{t_j}\int_0^t \beta(t-s)\big[A\check{u}(s) - A\bar{u}(s)\big]\,\mathrm{d}s\,\mathrm{d}t. \end{aligned} \tag{3.6}$$

In the following bound for the first of these integrals we allow for the possibility that $\|Au''(t)\|$ is not integrable on the first subinterval $(0, t_1)$.

Lemma 3.2 *For $\eta_{21}^{j-1/2}$ defined as in (3.6) we have*

$$\sum_{j=1}^n \left\|\eta_{21}^{j-1/2}\right\| k_j \le C_\alpha t_n^\alpha \left(\int_0^{t_1} t\|Au'(t)\|\,dt + \sum_{j=2}^n k_j^2 \int_{t_{j-1}}^{t_j} \|Au''(t)\|\,dt \right).$$

Proof Recall the notation $\omega_\mu = t^{\mu-1}/\Gamma(\mu)$ from the proof of Theorem 2.4, and note that $\beta = \omega_\alpha = \omega'_{1+\alpha}$ and $\omega_{1+\alpha}(0) = 0$. For $0 < s < t_1$,

$$u(s) - \check{u}(s) = u(s) - u(t_1) = -\int_s^{t_1} u'(\xi)\,\mathrm{d}\xi, \tag{3.7}$$

and therefore, changing the order of integration twice,

$$\begin{aligned} \left\|\eta_{21}^{1/2}\right\| k_1 &\le \int_0^{t_1}\int_0^t \beta(t-s)\int_s^{t_1} \|Au'(\xi)\|\,\mathrm{d}\xi\,\mathrm{d}s\,\mathrm{d}t \\ &= \int_0^{t_1}\int_s^{t_1} \omega'_{1+\alpha}(t-s)\,\mathrm{d}t\int_s^{t_1} \|Au'(\xi)\|\,\mathrm{d}\xi\,\mathrm{d}s \end{aligned}$$

$$= \int_0^{t_1} \omega_{1+\alpha}(t_1 - s) \int_s^{t_1} \|Au'(\xi)\| \, d\xi \, ds$$

$$\leq \omega_{1+\alpha}(t_1) \int_0^{t_1} \|Au'(\xi)\| \int_0^{\xi} ds \, d\xi \leq C_\alpha t_1^\alpha \int_0^{t_1} \xi \|Au'(\xi)\| \, d\xi.$$

For the sum over $j \geq 2$, we also change the order of integration,

$$\sum_{j=2}^{n} \left\| \eta_{21}^{j-1/2} \right\| k_j \leq \int_{t_1}^{t_n} \int_0^{t} \omega_\alpha(t-s) \|Au(s) - A\check{u}(s)\| \, ds \, dt$$

$$= \int_0^{t_1} \|Au(s) - A\check{u}(s)\| \int_{t_1}^{t_n} \omega'_{1+\alpha}(t-s) \, dt \, ds$$

$$+ \int_{t_1}^{t_n} \|Au(s) - A\check{u}(s)\| \int_s^{t_n} \omega'_{1+\alpha}(t-s) \, dt \, ds$$

$$\leq \omega_{1+\alpha}(t_n) \sum_{j=1}^{n} \int_{t_{i-1}}^{t_i} \|Au(s) - A\check{u}(s)\| \, ds.$$

To handle the term with $j = 1$ we argue as above with (3.7) to obtain

$$\int_0^{t_1} \|Au(s) - A\check{u}(s)\| \, ds \leq \int_0^{t_1} \xi \|Au'(\xi)\| \, d\xi.$$

For $j \geq 2$ we apply the Peano kernel theorem to obtain

$$u(s) - \check{u}(s) = \int_{t_{j-1}}^{t_j} \left[(s-\xi)_+ - k_j^{-1}(s - t_{j-1})(t_j - \xi) \right] u''(\xi) \, d\xi \quad \text{for } t_{j-1} < s < t_j,$$

where $(x-\xi)_+ = \max(x-\xi, 0)$, and deduce that

$$\int_{t_{j-1}}^{t_j} \|Au(s) - A\check{u}(s)\| \, ds \leq \int_{t_{j-1}}^{t_j} \int_{t_{j-1}}^{t_j} k_j \|Au''(\xi)\| \, d\xi \, ds$$

$$= k_j^2 \int_{t_{j-1}}^{t_j} \|Au''(\xi)\| \, d\xi.$$

□

To state the next theorem, we denote the midpoint of the interval $[t_{j-1}, t_{j+1}]$ by

$$t_j^* = \frac{t_{j+1} + t_{j-1}}{2} \quad \text{for } j \geq 2. \tag{3.8}$$

Theorem 3.3 *Let u be the solution of the initial value problem (1.2) and let U^n be the solution of the discrete-time scheme (1.8). If the time steps satisfy*

$$k_j \leq k_{j+1} \leq Ck_j \quad \textit{for all } j \geq 1,$$

then for $0 \leq t_n \leq T$,

$$\begin{aligned}
\|U^n - u(t_n)\| &\leq \|U^0 - u_0\| + 2\sum_{j=1}^{n} \left\| f^{j-1/2} k_j - \int_{t_{j-1}}^{t_j} f(t)\,dt \right\| \\
&\quad + C_{\alpha,T} \left(\int_0^{t_1} t\|Au'(t)\|\,dt + k_2 \int_{t_1}^{t_2} \|Au'(t)\|\,dt + \sum_{j=2}^{n} k_j^2 \int_{t_{j-1}}^{t_j} \|Au''(t)\|\,dt \right) \\
&\quad + C_{\alpha,T} \sum_{j=2}^{n-1} \left(k_j \int_{t_j}^{t_j^*} \|Au'(t)\|\,dt + (k_{j+1} - k_j) \int_{t_{j-1}}^{t_{j+1}} \|Au'(t)\|\,dt \right).
\end{aligned} \tag{3.9}$$

Proof It remains to estimate the contribution to the error from the second integral $\eta_{22}^{j-1/2}$ in (3.6). Letting $\Delta u^i = u(t_i) - u(t_{i-1})$, we find that

$$\check{u}(s) - \bar{u}(s) = \Delta u^i \,\frac{s - t_{i-1/2}}{k_i} \quad \text{for } t_{i-1} < s < t_i \text{ and } i \geq 2,$$

whereas $\check{u}(s) - \bar{u}(s) = 0$ for $0 < s < t_1$. Thus, $\eta_{22}^{1/2} = 0$ and, for $j \geq 2$,

$$\begin{aligned}
\eta_{22}^{j-1/2} k_j &= \int_{t_{j-1}}^{t_j} \sum_{i=2}^{j-1} \int_{t_{i-1}}^{t_i} \beta(t-s) A\Delta u^i \,\frac{s - t_{i-1/2}}{k_i}\,\mathrm{d}s\,\mathrm{d}t \\
&\quad + \int_{t_{j-1}}^{t_j} \int_{t_{j-1}}^{t} \beta(t-s) A\Delta u^j \,\frac{s - t_{j-1/2}}{k_j}\,\mathrm{d}s\,\mathrm{d}t
\end{aligned}$$

$$= \sum_{i=2}^{j-1} \frac{A\Delta u^i}{k_i} \int_{t_{j-1}}^{t_j} \int_{t_{i-1}}^{t_i} \omega_\alpha(t-s)(s-t_{i-1/2})\,\mathrm{d}s\,\mathrm{d}t$$

$$+ \frac{A\Delta u^j}{k_j} \int_{t_{j-1}}^{t_j} \int_{t_{j-1}}^{t} \omega_\alpha(t-s)(s-t_{j-1/2})\,\mathrm{d}s\,\mathrm{d}t.$$

After reversing the order of integration and using $\omega_\alpha = \omega'_{1+\alpha}$, we have

$$\eta_{22}^{j-1/2} k_j = \sum_{i=2}^{j-1} \frac{A\Delta u^i}{k_i} \int_{t_{i-1}}^{t_i} (s-t_{i-1/2})\big(\omega_{1+\alpha}(t_j-s) - \omega_{1+\alpha}(t_{j-1}-s)\big)\,\mathrm{d}s$$

$$+ \frac{A\Delta u^j}{k_j} \int_{t_{j-1}}^{t_j} (s-t_{j-1/2})\omega_{1+\alpha}(t_j-s)\,\mathrm{d}s,$$

and integration by parts shows that

$$\int_{t_{i-1}}^{t_i} (s-t_{i-1/2})\big(\omega_{1+\alpha}(t_j-s) - \omega_{1+\alpha}(t_{j-1}-s)\big)\,\mathrm{d}s$$

$$= \frac{k_i^2}{8}\big[\omega_{1+\alpha}(t_j-s) - \omega_{1+\alpha}(t_{j-1}-s)\big]_{s=t_{i-1}}^{t_i}$$

$$+ \frac{1}{2} \int_{t_{i-1}}^{t_i} (s-t_{i-1/2})^2\big(\omega_\alpha(t_j-s) - \omega_\alpha(t_{j-1}-s)\big)\,\mathrm{d}s$$

and

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

$$= -\frac{k_j^2}{8}\,\omega_{1+\alpha}(k_j) + \frac{1}{2}\int_{t_{j-1}}^{t_j} (s-t_{j-1/2})^2\omega_\alpha(t_j-s)\,\mathrm{d}s.$$

Thus, $\eta_{22}^{j-1/2} k_j = \frac{1}{8}B_1^j + \frac{1}{2}B_2^j$, where

$$B_1^j = -k_j\omega_{1+\alpha}(k_j)A\Delta u^j + \sum_{i=2}^{j-1} k_i A\Delta u^i\big[\omega_{1+\alpha}(t_j-s) - \omega_{1+\alpha}(t_{j-1}-s)\big]_{s=t_{i-1}}^{t_i},$$

$$B_2^j = \frac{A\Delta u^j}{k_j}\int_{t_{j-1}}^{t_j}(s-t_{j-1/2})^2\omega_\alpha(t_j-s)\,\mathrm{d}s$$
$$+\sum_{i=2}^{j-1}\frac{A\Delta u^i}{k_i}\int_{t_{i-1}}^{t_i}(s-t_{i-1/2})^2\big(\omega_\alpha(t_j-s)-\omega_\alpha(t_{j-1}-s)\big)\,\mathrm{d}s. \tag{3.10}$$

Using a shift of the summation index i, we find that

$$B_1^j = -k_2A\Delta u^2\big(\omega_{1+\alpha}(t_j-t_1)-\omega_{1+\alpha}(t_{j-1}-t_1)\big)$$
$$+\sum_{i=2}^{j-1}\big(k_iA\Delta u^i-k_{i+1}A\Delta u^{i+1}\big)\big(\omega_{1+\alpha}(t_j-t_i)-\omega_{1+\alpha}(t_{j-1}-t_i)\big),$$

and since $\omega_{1+\alpha}$ is an increasing function,

$$\sum_{j=2}^{n}\left\|B_1^j\right\| \le k_2\|A\Delta u^2\|\sum_{j=2}^{n}\big(\omega_{1+\alpha}(t_j-t_1)-\omega_{1+\alpha}(t_{j-1}-t_1)\big)$$
$$+\sum_{j=2}^{n}\sum_{i=2}^{j-1}\|k_iA\Delta u^i-k_{i+1}\Delta u^{i+1}\|\big(\omega_{1+\alpha}(t_j-t_i)-\omega_{1+\alpha}(t_{j-1}-t_i)\big).$$

After reversing the order of summation in the double sum, we see that the sums over j telescope to give

$$\sum_{j=2}^{n}\left\|B_1^j\right\| \le k_2\|A\Delta u^2\|\omega_{1+\alpha}(t_n-t_1)+\sum_{i=2}^{n-1}\|k_iA\Delta u^i-k_{i+1}A\Delta u^{i+1}\|\omega_{1+\alpha}(t_n-t_i)$$
$$\le \omega_{1+\alpha}(t_n)\left(k_2\|A\Delta u^2\|+\sum_{i=2}^{n-1}\|k_iA\Delta u^i-k_{i+1}A\Delta u^{i+1}\|\right). \tag{3.11}$$

To estimate (3.10), we make the splitting $B_2^j = B_{21}^j + B_{22}^j + B_{23}^j$ where

$$B_{21}^j = \sum_{i=3}^{j}\left(\frac{A\Delta u^i}{k_i}-\frac{A\Delta u^{i-1}}{k_{i-1}}\right)\int_{t_{i-1}}^{t_i}(s-t_{i-1/2})^2\omega_\alpha(t_j-s)\,\mathrm{d}s,$$

$$B_{22}^j = \sum_{i=3}^{j} \frac{A\Delta u^{i-1}}{k_{i-1}} \left(\int_{t_{i-1}}^{t_i} (s - t_{i-1/2})^2 \omega_\alpha(t_j - s)\, \mathrm{d}s - \int_{t_{i-2}}^{t_{i-1}} (s - t_{i-3/2})^2 \omega_\alpha(t_{j-1} - s)\, \mathrm{d}s \right), \tag{3.12}$$

$$B_{23}^j = \frac{A\Delta u^2}{k_2} \int_{t_1}^{t_2} (s - t_{3/2})^2 \omega_\alpha(t_j - s)\, \mathrm{d}s.$$

For the first of these quantities, we find that

$$\begin{aligned}\sum_{j=2}^{n} \left\| B_{21}^j \right\| &\le \sum_{j=2}^{n} \sum_{i=3}^{j} \left\| \frac{A\Delta u^i}{k_i} - \frac{A\Delta u^{i-1}}{k_{i-1}} \right\| \int_{t_{i-1}}^{t_i} (s - t_{i-1/2})^2 \omega_\alpha(t_j - s)\, \mathrm{d}s \\ &\le \sum_{i=3}^{n} \left\| \frac{A\Delta u^i}{k_i} - \frac{A\Delta u^{i-1}}{k_{i-1}} \right\| \frac{k_i^2}{4} \sum_{j=i}^{n} \int_{t_{i-1}}^{t_i} \omega_\alpha(t_j - s)\, \mathrm{d}s,\end{aligned}$$

and since $t_j - t_{i-1} = t_{j+1} - t_i - (k_{j+1} - k_i) \le t_{j+1} - t_i$ for $j \ge i$,

$$\begin{aligned}\sum_{j=i}^{n} \int_{t_{i-1}}^{t_i} \omega_\alpha(t_j - s)\, \mathrm{d}s &= \sum_{j=i}^{n} \big(\omega_{1+\alpha}(t_j - t_{i-1}) - \omega_{1+\alpha}(t_j - t_i) \big) \\ &\le \sum_{j=i}^{n} \big(\omega_{1+\alpha}(t_{j+1} - t_i) - \omega_{1+\alpha}(t_j - t_i) \big) = \omega_{1+\alpha}(t_{n+1} - t_i),\end{aligned} \tag{3.13}$$

so

$$\sum_{j=2}^{n} \left\| B_{21}^j \right\| \le \omega_{1+\alpha}(t_{n+1}) \sum_{i=3}^{n} \frac{k_i}{4k_{i-1}} \left\| k_{i-1} A\Delta u^i - k_i A\Delta u^{i-1} \right\|. \tag{3.14}$$

To deal with B_{22}^j, we let $s = [(t_i - s')t_{i-2} + (s' - t_{i-1})t_{i-1}]/k_i$ and obtain

$$\int_{t_{i-2}}^{t_{i-1}} (s - t_{i-3/2})^2 \omega_\alpha(t_{j-1} - s)\, \mathrm{d}s = \left(\frac{k_{i-1}}{k_i} \right)^3 \int_{t_{i-1}}^{t_i} (s' - t_{i-1/2})^2 \omega_\alpha\big(t_{j-1} - s\big)\, \mathrm{d}s'.$$

Observe that for $s' \le t_i$ and $i \le j$,

$$\begin{aligned} t_{j-1} - s &= t_j - k_j - k_i^{-1}\bigl(k_{i-1}s' + t_i t_{i-2} - t_{i-1}^2\bigr) \\ &= t_j - s' - k_j + k_i^{-1}\bigl((k_i - k_{i-1})s' + t_{i-1}^2 - t_i t_{i-2}\bigr) \\ &\le t_j - s' - k_j + k_i^{-1}\bigl((k_i - k_{i-1})t_i + t_{i-1}^2 - t_i t_{i-2}\bigr) = t_j - s' - (k_j - k_i), \end{aligned}$$

so $t_{j-1} - s \le t_j - s'$ and thus, since ω_α is a decreasing function,

$$\int_{t_{i-2}}^{t_{i-1}} (s - t_{i-3/2})^2 \omega_\alpha(t_{j-1} - s)\,\mathrm{d}s \ge \left(\frac{k_{i-1}}{k_i}\right)^3 \int_{t_{i-1}}^{t_i} (s' - t_{i-1/2})^2 \omega_\alpha(t_j - s')\,\mathrm{d}s'. \quad (3.15)$$

We therefore make a further splitting $B_{22}^j = B_{221}^j - B_{222}^j$, where

$$B_{221}^j = \sum_{i=3}^{j} \frac{A\Delta u^{i-1}}{k_{i-1}} \left(1 - \frac{k_{i-1}^3}{k_i^3}\right) \int_{t_{i-1}}^{t_i} (s - t_{i-1/2})^2 \omega_\alpha(t_j - s)\,\mathrm{d}s,$$

$$B_{222}^j = \sum_{i=3}^{j} \frac{A\Delta u^{i-1}}{k_{i-1}} \left(\int_{t_{i-2}}^{t_{i-1}} (s - t_{i-3/2})^2 \omega_\alpha(t_{j-1} - s)\,\mathrm{d}s - \frac{k_{i-1}^3}{k_i^3} \int_{t_{i-1}}^{t_i} (s - t_{i-1/2})^2 \omega_\alpha(t_j - s)\,\mathrm{d}s \right).$$

Observing that

$$\begin{aligned} \sum_{j=2}^{n} \left\| B_{221}^j \right\| &\le \sum_{j=2}^{n} \sum_{i=3}^{j} \frac{\|A\Delta u^{i-1}\|}{k_{i-1}} \left(1 - \frac{k_{i-1}^3}{k_i^3}\right) \int_{t_{i-2}}^{t_{i-1}} (s - t_{i-1/2})^2 \omega_\alpha(t_j - s)\,\mathrm{d}s \\ &\le \sum_{i=3}^{n} \frac{k_i^3 - k_{i-1}^3}{k_{i-1}k_i^3} \|A\Delta u^{i-1}\| \frac{k_i^2}{4} \sum_{j=i}^{n} \int_{t_{i-1}}^{t_i} \omega_\alpha(t_j - s)\,\mathrm{d}s, \end{aligned}$$

and after applying (3.13) and using

$$\frac{k_i^3 - k_{i-1}^3}{k_i k_{i-1}} = \frac{k_i^2 + k_i k_{i-1} + k_{i-1}^2}{k_i k_{i-1}} (k_i - k_{i-1}) \le C(k_i - k_{i-1}),$$

we have

$$\sum_{j=2}^{n} \left\| B_{221}^j \right\| \le C\omega_{1+\alpha}(t_{n+1}) \sum_{i=3}^{n} (k_i - k_{i-1}) \|A\Delta u^{i-1}\|. \quad (3.16)$$

The inequality (3.15) implies that

$$\sum_{j=2}^{n} \left\| B_{222}^{j} \right\| \leq \sum_{i=3}^{n} \frac{\|A\Delta u^{i-1}\|}{k_{i-1}} \sum_{j=i}^{n} \left(\int_{t_{i-2}}^{t_{i-1}} (s - t_{i-3/2})^2 \omega_\alpha(t_{j-1} - s)\, ds - \frac{k_{i-1}^3}{k_i^3} \int_{t_{i-1}}^{t_i} (s - t_{i-1/2})^2 \omega_\alpha(t_j - s)\, ds \right),$$

and a shift of the indices gives

$$\sum_{j=2}^{n} \left\| B_{222}^{j} \right\| \leq \sum_{i=2}^{n-1} \frac{\|A\Delta u^{i}\|}{k_i} \sum_{j=i}^{n-1} \int_{t_{i-1}}^{t_i} (s - t_{i-1/2})^2 \omega_\alpha(t_j - s)\, ds - \sum_{i=3}^{n} \frac{\|A\Delta u^{i-1}\|}{k_{i-1}} \frac{k_{i-1}^3}{k_i^3} \sum_{j=i}^{n} \int_{t_{i-1}}^{t_i} (s - t_{i-1/2})^2 \omega_\alpha(t_j - s)\, ds.$$

With the help of (3.13), it follows that

$$\begin{aligned} \sum_{j=2}^{n} \left\| B_{222}^{j} \right\| &\leq \frac{\|A\Delta u^2\|}{k_2} \frac{k_2^2}{4} \sum_{j=2}^{n} \int_{t_1}^{t_2} \omega_\alpha(t_j - s)\, ds \\ &\quad + \sum_{i=3}^{n-1} \left| \frac{\|A\Delta u^i\|}{k_i} - \frac{\|A\Delta u^{i-1}\|}{k_{i-1}} \frac{k_{i-1}^3}{k_i^3} \right| \frac{k_i^2}{4} \sum_{j=i}^{n-1} \int_{t_{i-1}}^{t_i} \omega_\alpha(t_j - s)\, ds \\ &\leq \frac{1}{4} \omega_{1+\alpha}(t_n) \left(k_2 \|A\Delta u^2\| + \sum_{i=3}^{n-1} k_i^{-1} \left\| k_i^2 A\Delta u^i - k_{i-1}^2 A\Delta u^{i-1} \right\| \right). \end{aligned} \tag{3.17}$$

For the remaining quantity in (3.12),

$$\sum_{j=2}^{n} \left\| B_{23}^{j} \right\| \leq \frac{\|A\Delta u^2\|}{k_2} \frac{k_2^2}{4} \sum_{j=2}^{n} \int_{t_1}^{t_2} \omega_\alpha(t_j - s)\, ds \leq \frac{1}{4} \omega_{1+\alpha}(t_{n+1} - t_1) k_2 \|A\Delta u^2\|, \tag{3.18}$$

and so, putting

$$\begin{aligned}\delta_j &= \left\|k_j A\Delta u^j - k_{j+1} A\Delta u^{j+1}\right\| + \left\|k_j A\Delta u^{j+1} - k_{j+1} A\Delta u^j\right\| + (k_{j+1}-k_j)\|A\Delta u^j\| \\ &\quad + k_{j+1}^{-1}\left\|k_{j+1}^2 A\Delta u^{j+1} - k_j^2 A\Delta u^j\right\| \\ &\le 3k_j\left\|A(\Delta u^{j+1}-\Delta u^j)\right\| + (k_{j+1}-k_j)\big(3\|A\Delta u^{j+1}\| + 2\|A\Delta u^j\|\big),\end{aligned}$$

we see that the estimates (3.11), (3.14), (3.16), (3.17) and (3.18) above give

$$\sum_{j=2}^{n}\left\|\eta_{22}^j\right\| k_j \le C_{\alpha,T}\left(k_2\|A\Delta u^2\| + \sum_{j=2}^{n-1}\delta_j\right). \tag{3.19}$$

Recall from (3.8) that t_j^* denotes the midpoint of the interval $[t_{j-1}, t_{j+1}]$, and define $\Delta^2 u^j = u(t_{j+1}) - 2u(t_j^*) + u(t_{j-1})$. Since $\Delta^2 u^j = 0$ if $u(t)$ is a polynomial of degree at most 1, the Peano kernel theorem implies that

$$\Delta^2 u_j = \int_{t_{j-1}}^{t_j} K_j(t)u''(t)\,\mathrm{d}t \qquad \text{where} \quad K_j(t) = \begin{cases} t - t_{j-1} & \text{for } t_{j-1} < t < t_j^*, \\ t_{j+1} - t & \text{for } t_j^* < t < t_{j+1}, \end{cases}$$

and we see that $|K_j(t)| \le \frac{1}{2}(k_j + k_{j+1})$ for $t_{j-1} < t < t_{j+1}$. By assumption $k_j \le k_{j+1}$ so $t_j^* \ge t_j$ and we have

$$\begin{aligned}\left\|A(\Delta u^{j+1} - \Delta u^j)\right\| &\le \|A\Delta^2 u^j\| + 2\|Au\left(t_j^*\right) - Au(t_j)\| \\ &\le k_j \int_{t_{j-1}}^{t_{j+1}} \|Au''(t)\|\,\mathrm{d}t + 2\int_{t_j}^{t_j^*}\|Au'(t)\|\,\mathrm{d}t.\end{aligned}$$

Thus, δ_j is bounded by

$$3k_j^2\int_{t_{j-1}}^{t_{j+1}}\|Au''(t)\|\,\mathrm{d}t + 6k_j\int_{t_j}^{t_j^*}\|Au'(t)\|\,\mathrm{d}t + 3(k_{j+1}-k_j)\int_{t_{j-1}}^{t_{j+1}}\|Au'(t)\|\,\mathrm{d}t,$$

and the error bound (3.9) follows from (3.19) using $\|A\Delta u^2\| \le \int_{t_1}^{t_2}\|Au'(t)\|\,\mathrm{d}t$. □

We now show how the error depends on the mesh grading parameter $\gamma \ge 1$.

Corollary 3.4 *Assume that the t_n satisfy* (1.9), (1.10) *and* (1.11), *and that the $f^{n-1/2}$ satisfy* (1.6) *and* (1.7). *If the exact solution and the source term satisfy*

$$t\|Au'(t)\| + t^2\|Au''(t)\| \le Mt^{\sigma-1} \quad \textit{and} \quad t\|f'(t)\| + t^2\|f''(t)\| \le Mt^{\sigma-1}$$

for $t > 0$*, with* $\sigma > 0$*, then for* $0 \le t_n \le T$*,*

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

Proof We see that

$$\left\| f^{1/2}\, k_1 - \int_0^{t_1} f(t)\,\mathrm{d}t \right\| \le C \int_0^{t_1} t\|f'(t)\|\,\mathrm{d}t \le C_\sigma M t_1^\sigma \le C_{\sigma,\gamma} M k^{\gamma\sigma}$$

and, for $j \ge 2$,

$$\begin{aligned} \left\| f^{j-1/2}\, k_j - \int_{t_{j-1}}^{t_j} f(t)\,\mathrm{d}t \right\| &\le C k_j^2 \int_{t_{j-1}}^{t_j} \|f''(t)\|\,\mathrm{d}t \\ &\le C M t_j^{\sigma-3}\, k_j^3 \le C_\gamma M k^2 t_j^{\sigma-2/\gamma-1} k_j. \end{aligned}$$

Using $t_1^{-1} k_2 \le C_\gamma t_1^{-1} k t_2^{1-1/\gamma} \le C_\gamma k t_1^{-1/\gamma} \le C_\gamma$ we have

$$\begin{aligned} \int_0^{t_1} t\|Au'(t)\|\,dt + k_2 \int_{t_1}^{t_2} \|Au'(t)\|\,\mathrm{d}t &\le C_\sigma M \big(t_1^\sigma + t_1^{\sigma-1} k_2\big) \\ &\le C_{\sigma,\gamma} M t_1^\sigma \le C_{\sigma,\gamma} M k^{\gamma\sigma}, \end{aligned}$$

and since $t_j^* - t_j = \frac{1}{2}(k_{j+1} - k_j)$, our assumptions on the mesh imply that for $j \ge 2$,

$$\begin{aligned} & k_j^2 \int_{t_{j-1}}^{t_j} \|Au''(t)\|\,\mathrm{d}t + k_j \int_{t_j}^{t_j^*} \|Au'(t)\|\,\mathrm{d}t + (k_{j+1} - k_j) \int_{t_{j-1}}^{t_{j+1}} \|Au'(t)\|\,\mathrm{d}t \\ &\le C_\sigma \Big(k_j^2 t_j^{\sigma-3} k_j + k_j (t_j^* - t_j) t_j^{\sigma-2} + (k_{j+1} - k_j) t_j^{\sigma-2} (k_j + k_{j+1}) \Big) \\ &\le C_{\sigma,\gamma} M k^2 t_j^{\sigma-2/\gamma-1} k_j. \end{aligned}$$

Thus, we estimate the sum

$$\sum_{j=2}^{n} t_j^{\sigma-2/\gamma-1} k_j \le C_{\sigma,\gamma} \int_{t_1}^{t_n} t^{\sigma-2/\gamma-1}\,\mathrm{d}t$$

$$\le C_{\sigma,\gamma} \times \begin{cases} t_1^{\sigma-2/\gamma}/(2/\gamma-\sigma) & \text{if } \sigma < 2/\gamma, \\ \log(t_n/t_1) & \text{if } \sigma = 2/\gamma, \\ t_n^{\sigma-2/\gamma}/(\sigma-2/\gamma) & \text{if } \sigma > 2/\gamma. \end{cases}$$

The result follows after noting that, in the first case,

$$t_1^{\sigma-2/\gamma} = (k_1)^{-(2/\gamma-\sigma)} \le (c_\gamma k^\gamma)^{-(2/\gamma-\sigma)} = C_{\sigma,\gamma} k^{\gamma\sigma-2}.$$

□

Example 3.5 If $u_0 \in \dot{H}^2$ and $f \in \dot{H}^{2\alpha/(1+\alpha)}$, then by Corollaries 2.2 and 2.5 we may take $\sigma = 1$, so the error is $O(k^\gamma)$ if $1 \le \gamma < 2$, $O(k^2|\log k|)$ if $\gamma = 2$, and $O(k^2)$ if $\gamma > 2$.

4 Discretization in space

Using the bilinear form (2.3) associated with A, we write the weak form of the initial value problem (1.2) as

$$\left\langle \frac{\partial u}{\partial t}, \chi \right\rangle + \int_0^t \beta(t-s)\mathsf{A}\big(u(s),\chi\big)\,\mathrm{d}s = \big\langle f(t),\chi\big\rangle \quad \text{for } t>0 \text{ and } \chi \in \dot{H}^1.$$

For our spatially-discrete numerical scheme, we choose a finite-dimensional subspace $V_h \subseteq \dot{H}^1$ and seek $U_h^n \in V_h$ that satisfies

$$\left\langle \frac{U_h^n - U_h^{n-1}}{k_n}, \chi \right\rangle + \mathscr{I}_\alpha^{n-1/2}\mathsf{A}(U_h,\chi) = \langle f^{n-1/2},\chi\rangle \quad \text{for } n \ge 1 \text{ and } \chi \in V_h, \tag{4.1}$$

starting from a suitable approximation $U_h^0 \approx u_0$. The same energy argument used to prove Theorem 3.1 shows that the scheme (4.1) is unconditionally stable:

$$\|U_h^n\| \le \|U_h^0\| + 2\sum_{j=1}^{n} \|f^{n-1/2}\|\,k_j \quad \text{for } n \ge 1. \tag{4.2}$$

Now let $\mathbb{H} = L_2(\Omega)$ for a bounded, convex or $C^{1,1}$ domain $\Omega \subseteq \mathbb{R}^d$ and assume that A is a strongly elliptic, second-order linear partial differential operator satisfying our earlier assumptions. We further assume the approximation property

$$\min_{\chi \in V_h} \|v - \chi\| \le Ch^\kappa \|v\|_k \quad \text{for } v \in \dot{H}^\kappa \text{ and } 0 \le \kappa \le 2. \tag{4.3}$$

Thus, in particular, V_h may be a continuous, piecewise-linear finite element space constructed on a triangulation of Ω for which h is the maximum element diameter. To state our error bound for the space discretization, we let $R_h : \dot{H}^1 \to V_h$ denote the Ritz projector for the modified (strictly positive-definite) operator $A + I$. Thus,

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

and we recall that

$$\|v - R_h v\| \le Ch^\kappa \|v\|_\kappa \quad \text{for } 0 \le \kappa \le 2. \tag{4.4}$$

The error bound in the next theorem allows for the possibility that $\|u'(t)\|_\kappa$ is not integrable on the first subinterval $(0, t_1)$.

Theorem 4.1 *Assume that V_h has the approximation property (4.3), let u be the solution of the intial value problem (1.2) and let $U_h^n \in V_h$ be the solution of the discrete-time, discrete-space scheme (4.1). The error bound of Theorem 3.3 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*

$$\|U_h^0 - R_h u_0\| + C_{\alpha,T} h^\kappa \left(\|u_0\|_\kappa + \|u(t_1)\|_\kappa + \int_{t_1}^{t_n} \|u'(t)\|_\kappa \, \mathrm{d}t \right) \quad \textit{for } 0 \le \kappa \le 2. \tag{4.5}$$

Proof The proof is similar to [14, Theorems 3.1 and 3.2]. We write $U_h^n - u(t_n) = \theta^n + \rho(t_n)$ where $\theta^n = U_h^n - R_h u(t_n) \in V_h$ and $\rho(t) = R_h u(t) - u(t)$, and find that

$$\langle \theta^n - \theta^{n-1}, \chi\rangle + \int_{t_{n-1}}^{t_n} \int_0^t \beta(t-s) \mathsf{A}\big(\bar{\theta}(s), \chi\big) \, \mathrm{d}s \, \mathrm{d}t = \langle \eta^{n-1/2}, \chi\rangle \, k_n \quad \text{for } \chi \in V_h.$$

Here, $\eta^{n-1/2} = \eta_1^{n-1/2} + \eta_2^{n-1/2} + \eta_3^{n-1/2} + \eta_4^{n-1/2}$, for the same $\eta_1^{n-1/2}$ and $\eta_2^{n-1/2}$ as in (3.4) and for

$$\eta_3^{n-1/2} = \frac{1}{k_n} \int_{t_{n-1}}^{t_n} \int_0^t \beta(t-s) \bar{\rho}(s) \, \mathrm{d}s \, \mathrm{d}t,$$

$$\eta_4^{n-1/2} = -\frac{1}{k_n} \big[\rho(t_n) - \rho(t_{n-1})\big].$$

The error bound follows by applying the stability estimate (4.2) to θ^n, together with the results of Theorem 3.3 and the error bound (4.4) for the Ritz projector; the details are given in the preprint [13, Theorem 5.1]. □

Corollary 4.2 *Let* $0 \le \kappa \le 2$. *If the exact solution of* (1.2) *satisfies*

$$\|u(t)\|_\kappa + t\|u'(t)\|_\kappa \le Mt^\nu \quad \text{for } t > 0, \text{ with } \nu \ge 0,$$

then the error terms (4.5) *due to the spatial discretization are bounded by*

$$\|U_h^0 - R_h u_0\| + C_{\alpha,T,\nu} M h^\kappa \times \begin{cases} 1 + \log(t_n/t_1) & \text{if } \nu = 0, \\ 1 & \text{if } \nu > 0. \end{cases}$$

5 Numerical experiments

In this section, we apply our fully-discrete Crank-Nicolson scheme (4.1) to a concrete problem of the form (1.2) in one space dimension, taking $\alpha = \frac{1}{2}$, $T = 1$ and $Au = -u_{xx}$ on the interval $\Omega = (0, 1)$ with homogeneous Neumann boundary conditions $u_x(0, t) = 0 = u_x(1, t)$ for $0 \le t \le T$. We employ a time mesh of the form (1.12) and a uniform spatial mesh with N subintervals of length $h = 1/N$. Since N is the same for the space and time meshes, this means $h = k$. For the finite element space V_h we choose the space of continuous, piecewise-linear functions, and for U_h^0 we choose the L_2 projection of the initial data u_0 onto V_h. The data are chosen so that the exact solution is

$$u(x, t) = \cos(\pi x) - \frac{4t^{3/2}}{3\sqrt{\pi}}\big(1 + \cos(2\pi x)\big), \tag{5.1}$$

i.e., $f(x, t) = 2\pi^{3/2}t^{1/2}\cos(\pi x) - 2\pi^{-1/2}t^{1/2}\big(1 + \cos(2\pi x)\big) - 2\pi^2 t^2 \cos(2\pi x)$ and $u_0(x) = \cos(\pi x)$. Thus, for $t > 0$,

$$t\|Au'(t)\| + t^2\|Au''(t)\| \le Mt^{3/2} \quad \text{and} \quad t\|f'(t)\| + t^2\|f''(t)\| \le Mt^{1/2},$$

so the assumptions of Corollaries 3.4 and 4.2 are satisfied for $\sigma = 3/2$, $\nu = 0$ and $\kappa = 2$. Table 1 shows the maximum $L_2(\Omega)$-error, $\max_{0\le n\le N}\|U_h^n - u(t_n)\|$, when $f^{n-1/2} = f(t_{n-1/2})$. As predicted, the observed convergence rate is roughly $O(k^{3/2} + h^2|\log k|) = O(N^{-3/2})$ for uniform time steps, i.e., for $\gamma = 1$, but this rate improves to $O(N^{-2}\log N)$ if $\gamma = 2/\sigma = 4/3$. For $\gamma = 2$ the mesh is over-graded: theoretically, we have a slightly better convergence rate of $O(N^{-2})$ but in practice the errors are larger than when $\gamma = 4/3$.

Space limitations prevent us from showing more tables, but we will comment briefly on the results of some other numerical investigations.

By using the exact integral $f^{n-1/2} = \frac{1}{k_n}\int_{t_{n-1}}^{t_n} f(t)\,dt$ of the source term, we can eliminate the influence of the singular behaviour of $f(t)$ on the error bound of

Table 1 Maximum $L_2(\Omega)$-errors and apparent convergence rates for three different mesh gradings when $f^{n-1/2} = f(t_{n-1/2})$ and the exact solution is (5.1)

N	$\gamma = 1$		$\gamma = 4/3$		$\gamma = 2$	
20	5.42e-03		5.53e-03		6.37e-03	
40	1.39e-03	1.95	1.39e-03	1.99	1.63e-03	1.99
80	5.17e-04	1.43	3.47e-04	1.99	4.00e-04	1.99
160	1.95e-04	1.40	8.14e-05	2.09	9.54e-05	2.07
320	7.26e-05	1.42	2.04e-05	1.99	2.39e-05	1.99

Corollary 3.4, allowing us to take $\sigma = 5/2$, and thereby achieve second-order accuracy even for a uniform time mesh.

By discretizing in space only, we obtain an approximate solution $u_h(t)$ satisfying $\|u(t) - u_h(t)\|_{H^1(\Omega)} = O(h)$; see [14, Theorem 2.2]. Thus, we might expect $\|U_h^n - u(t_n)\|_{H^1(\Omega)}$ to be $O(k^{3/2} + h)$ if $\gamma = 1$, $O(k^2|\log k| + h)$ if $\gamma = 4/3$ and $O(k^2 + h)$ if $\gamma = 2$. For $h = k$, the error from the spatial discretization dominates in each case, giving $O(h) = O(N^{-1})$, which is exactly what we observed in practice. In fact, the H^1-errors are almost independent of the mesh grading.

Finally, we investigated a modified time mesh

$$t'_n = \begin{cases} t_n - \theta k_n & \text{for } n = 1, 3, 5, \ldots, N-1, \\ t_n + \theta k_{n+1} & \text{for } n = 2, 4, 6, \ldots, N-2, \end{cases} \tag{5.2}$$

where t_n is the smoothly-graded mesh (1.12) used above and θ is a fixed parameter in the range $0 \le \theta < 1/2$. The first and last points are unchanged: $t'_0 = 0 = t_0$ and $t'_N = T = t_N$. The subintervals of the modified mesh (5.2) are alternately shorter or longer than the ones of the original mesh (1.12), with $k'_1 = (1-\theta)k_1$,

$$k'_n = t'_n - t'_{n-1} = \begin{cases} k_n - 2\theta k_n & \text{for } n = 3, 5, \ldots, N-1 \\ k_n + \theta(k_{n+1} + k_n) & \text{for } n = 2, 4, \ldots, N-2, \end{cases}$$

and $k'_N = k_N + \theta k_{N-1}$. Thus, the modified mesh satisfies the basic assumptions (1.9) and (1.10), but not the more restrictive condition (1.11). In practice, however, we found that the convergence behaviour was not sensitive to the choice of θ, suggesting that the time discretization scheme (1.8) is more robust than our analysis is able to show.

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