Time-stepping error bounds for fractional diffusion problems with non-smooth initial data

William McLean\textsuperscript{a,1,2}, Kassem Mustapha\textsuperscript{b,1}

\textsuperscript{a}School of Mathematics and Statistics, The University of New South Wales, Sydney 2052, Australia
\textsuperscript{b}Department of Mathematics and Statistics, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia

Abstract

We apply the piecewise constant, discontinuous Galerkin method to discretize a fractional diffusion equation with respect to time. Using Laplace transform techniques, we show that the method is first order accurate at the \(n\)th time level \(t_n\), but the error bound includes a factor \(t_n^{-1}\) if we assume no smoothness of the initial data. We also show that for smoother initial data the growth in the error bound as \(t_n\) decreases is milder, and in some cases absent altogether. Our error bounds generalize known results for the classical heat equation and are illustrated for a model problem.

Keywords: Discontinuous Galerkin method, implicit Euler method, Laplace transform, polylogarithm.

2010 MSC: 65M15, 35R11, 45K05, 44A10.

1. Introduction

Consider an initial-value problem for an abstract, time-fractional diffusion equation [7, p. 84]

\[
\partial_t u + \partial_t^{1-\nu} Au = 0 \quad \text{for } t > 0, \quad \text{with } u(0) = u_0 \text{ and } 0 < \nu < 1.
\]

Here, we think of the solution \(u\) as a function from \([0, \infty)\) to a Hilbert space \(\mathcal{H}\), with \(\partial_t u = u'(t)\) the usual derivative with respect to \(t\), and with

\[
\partial_t^{1-\nu} u(t) = \frac{\partial}{\partial t} \int_0^t \frac{(t-s)^{\nu-1}}{\Gamma(\nu)} u(s) \, ds
\]
the Riemann–Liouville fractional derivative of order $1 - \nu$. The linear operator $A$ is assumed to be self-adjoint, positive-semidefinite and densely defined in $\mathcal{H}$, with a complete orthonormal eigensystem $\phi_1, \phi_2, \phi_3, \ldots$. We further assume that the eigenvalues of $A$ tend to infinity. Thus,

$$A\phi_m = \lambda_m \phi_m, \quad \langle \phi_m, \phi_n \rangle = \delta_{mn}, \quad 0 \leq \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots,$$

where $\langle u, v \rangle$ is the inner product in $\mathcal{H}$; the corresponding norm in $\mathcal{H}$ is denoted by $\|u\| = \sqrt{\langle u, u \rangle}$. In particular, we may take $Au = -\nabla^2 u$ and $\mathcal{H} = L^2(\Omega)$ for a bounded spatial domain $\Omega$, with $u$ subject to homogeneous Dirichlet or Neumann boundary conditions on $\partial \Omega$. Our problem (1) then reduces to the classical heat equation when $\nu \to 1$.

Many authors have studied techniques for the time discretization of (1), but obtaining sharp error bounds has proved challenging. In studies of explicit and implicit finite difference schemes [1, 3, 8, 14, 17, 20] the error analyses typically assume that the solution $u(t)$ is sufficiently smooth, including at $t = 0$, which amounts to imposing compatibility conditions on the initial data and source term. In our earlier work on discontinuous Galerkin (DG) time-stepping [11, 15, 16], we permitted more realistic behaviour, allowing the derivatives of $u(t)$ to be unbounded as $t \to 0$, but were seeking error bounds that are uniform in $t$ using variable time steps. In the present work, we again consider a piecewise-constant DG scheme but with a completely different method of analysis that leads to sharp error bounds even for non-smooth initial data, at the cost of requiring a constant time step $\Delta t$. Our previous analysis [11, Theorem 5] of the scheme (5), in conjunction with relevant estimates [10] of the derivatives of $u$, shows, in the special case of uniform time steps, only the sub-optimal error bound

$$\|U^n - u(t_n)\| \leq C\Delta t^\nu \|A^r u_0\| \quad \text{for} \quad 0 \leq r < 1/\nu. \quad (2)$$

In our main result, we substantially improve on (2) by showing that

$$\|U^n - u(t_n)\| \leq C\Delta t^{\nu-1} \|A^r u_0\| \quad \text{for} \quad 0 \leq r \leq \min(2, 1/\nu). \quad (3)$$

Thus, for a general $u_0 \in \mathcal{H}$ the error is of order $t_n^{-1} \Delta t$ at $t = t_n$, so the method is first-order accurate but the error bound includes a factor $t_n^{-1}$ that grows if $t_n$ approaches zero, until at $t = t_1$ the bound is of order $t_1^{-1} \Delta t = 1$. However, if $1/2 \leq \nu < 1$ and $u_0$ is smooth enough to belong to $D(A^{1/\nu})$, the domain of $A^{1/\nu}$, then the error is of order $\Delta t$, uniformly in $t_n$. For $0 < \nu \leq 1/2$, no matter how smooth $u_0$ a factor $t_n^{2\nu-1}$ is present. To the best of our knowledge, only Cuesta et al. [2] and McLean and Thomée [12, Theorem 3.1] have hitherto investigated the time discretization of (1) for the interesting case when the initial data might not be regular, the former using a finite difference-convolution quadrature scheme and the latter a method based on numerical inversion of the Laplace transform.

In the present work, we do not discuss the spatial discretization of (1). By contrast, Jin, Lazarov and Zhou [6] applied a piecewise linear finite element method using a quasi-uniform partition of $\Omega$ into elements with maximum diameter $h$, but with no time discretization. They worked with an equivalent
formulation of the fractional diffusion problem,
\[ \partial_t^{\nu} u - \nabla^2 u = 0 \quad \text{for} \quad x \in \Omega \text{ and } 0 < t \leq T, \quad (4) \]
where \( \partial_t^{\nu} \) denotes the Caputo fractional derivative, and proved [6, Theorems 3.5 and 3.7] that, for an appropriate choice of \( u_h(0) \),
\[ \|u_h(t) - u(t)\| + h\|\nabla (u_h - u)\| \leq Ct^{\nu(r-1)} \times \begin{cases} h^2\ell_h \|A^r u_0\|, & r \in \{0, 1/2\}, \\ h^2\|A^r u_0\|, & r = 1, \end{cases} \]
where \( \ell_h = \max(1, \log h^{-1}) \). These estimates for the spatial error complement our bounds for the error in a time discretization.

For a fixed step size \( \Delta t > 0 \), we put \( t_n = n\Delta t \) and define a piecewise-constant approximation \( U(t) \approx u(t) \) by applying the DG method [11, 13],
\[ U_n - U_{n-1} + \int_{t_{n-1}}^{t_n} \partial_t^{1-\nu} A U(t) \, dt = 0 \quad \text{for} \quad n \geq 1, \quad \text{with} \quad U^0 = u_0, \quad (5) \]
where \( U^n = U(t^+_n) = \lim_{t \rightarrow t^+_n} U(t) \) denotes the one-sided limit from below at the \( n \)th time level. Thus, \( U(t) = U^n \) for \( t_{n-1} < t \leq t_n \). Since we do not consider any spatial discretization, \( U \) is a semidiscrete solution with values in \( H \). A short calculation reveals that
\[ \int_{t_{n-1}}^{t_n} \partial_t^{1-\nu} A U(t) \, dt = \Delta t^{\nu} \sum_{j=1}^{n} \beta_{n-j} A U^j, \]
with
\[ \beta_0 = \Delta t^{-\nu} \int_{t_{n-1}}^{t_n} (t_n - t)^{\nu-1} t_{n-1}^{-\nu} dt = \frac{1}{\Gamma(1+\nu)} \]
and, for \( j \geq 1 \),
\[ \beta_j = \Delta t^{-\nu} \int_{t_{n-j-1}}^{t_{n-j}} (t_n - t)^{\nu-1} - (t_{n-1} - t)^{\nu-1} t_{n-1}^{-\nu} dt = \frac{(j+1)^{\nu} - 2j^{\nu} + (j-1)^{\nu}}{\Gamma(1+\nu)}. \]
Thus, by solving the recurrence relation
\[ (I + \beta_0 \Delta t^{\nu} A) U^n = U^{n-1} - \Delta t^{\nu} \sum_{j=1}^{n-1} \beta_{n-j} A U^j \quad (6) \]
for \( n = 1, 2, 3, \ldots \) we may compute \( U^1, U^2, U^3, \ldots \).

In the classical limit as \( \nu \rightarrow 1 \), the fractional-order equation (1) reduces to an abstract heat equation,
\[ \partial_t u + Au = 0 \quad \text{for} \quad t > 0, \quad \text{with} \quad u(0) = u_0, \quad (7) \]
and the time-stepping DG method (5) reduces to the implicit Euler scheme
\[ \frac{U^n - U^{n-1}}{\Delta t} + AU^n = 0, \quad (8) \]
for which the following error bound holds \cite[Theorems 7.1 and 7.2]{Thomee18}:

\[
\| U^n - u(t_n) \| \leq C \tau^{-r} t_n^n \| A^r u_0 \| \quad \text{for } n = 1, 2, 3, \ldots \text{ and } 0 \leq r \leq 1.
\] (9)

This result is just the limiting case as \( \nu \to 1 \) of our error estimate (3) for the fractional diffusion equation.

For any real \( r \geq 0 \), we can characterize \( D(A^r) \) in terms of the generalized Fourier coefficients in an eigenfunction expansion,

\[
v = \sum_{m=1}^{\infty} v_m \phi_m, \quad v_m = \langle v, \phi_m \rangle.
\]

Indeed, \( v \in \mathcal{H} \) belongs to \( D(A^r) \) if and only if

\[
\| A^r v \|_2^2 = \sum_{m=1}^{\infty} \lambda_m^{2r} v_m^2 < \infty,
\] (10)

in which case the series \( A^r v = \sum_{m=1}^{\infty} \lambda_m^r v_m \phi_m \) converges in \( \mathcal{H} \). Thus (recalling our assumption that \( \lambda_m \to \infty \)) the larger the value of \( r \) such that \( v \in D(A^r) \), the faster the Fourier coefficients \( v_m \) decay as \( m \to \infty \) and the “smoother” \( v \) is. When \( \mathcal{H} = L^2(\Omega) \) the functions in \( D(A^r) \) may have to satisfy compatibility conditions on \( \partial \Omega \); see Thomee \cite[Lemma 3.1]{Thomee18} or \cite[Section 3]{Thomee10}. In particular, an infinitely differentiable function will be somewhat “non-smooth” if it fails to satisfy the boundary conditions of our problem.

We note that, for a given \( u_0 \), the exact solution \( u \) is less smooth than is the case for the classical heat equation. To see why, consider the Fourier expansion

\[
u(t) = \sum_{m=1}^{\infty} u_m(t) \phi_m, \quad u_m(t) = \langle u(t), \phi_m \rangle,
\] (11)

and put \( u_{0m} = \langle u_0, \phi_m \rangle \). The Fourier coefficients \( u_m(t) \) satisfy the initial-value problem

\[
u_m + \lambda_m \partial_1^{1-\nu} u_m = 0, \quad \text{for } t > 0, \text{ with } u_m(0) = u_{0m},
\] (12)

so that, as is well known \cite{Thomee10}, \( u_m(t) = E_{\nu}(-\lambda_m t^\nu) u_{0m} \) where \( E_{\nu} \) denotes the Mittag-Leffler function. Since \( E_{\nu}(-s) = O(s^{-1}) \) decays slowly as \( s \to \infty \) for \( 0 < \nu < 1 \), in comparison to \( E_1(-s) = e^{-s} \), the high frequency modes of the solution are not damped as rapidly as in the classical case \( \nu = 1 \).

Section 2 uses Laplace transform techniques to derive integral representations for the Fourier coefficients \( U^n_m = \langle U^n, \phi_m \rangle \) and \( u_m(t_n) = \langle u(t_n), \phi_m \rangle \). We show that \( U^n_m - u_m(t_n) = \delta^n(\mu) u_{0m} \), where \( \delta^n(\mu) \) is given by an explicit but complicated integral; thus, the error has a Fourier expansion of the form

\[
u^n - u(t_n) = \sum_{m=1}^{\infty} \delta^n(\lambda_m \Delta^\nu) u_{0m} \phi_m, \quad u_{0m} = \langle u_0, \phi_m \rangle.
\] (13)

Theorem 4 states a key estimate for \( \delta^n(\mu) \), but to avoid a lengthy digression the proof is relegated to Section 4.
The main result (3) of the paper is established in Section 3, where we first prove in Theorem 5 that if $u_0 \in \mathcal{H}$ then the error is of order $t_n^{-1} \Delta t$, coinciding with the error estimate (9) for the classical heat equation when $r = 0$. Next we prove the special case $r = \min(2, 1/\nu)$ of (3) and then, in Theorem 7, deduce the general case by interpolation. The paper concludes with Section 5, which presents the results of some computational experiments for a model 1D problem, as well as numerical evidence that the constant $C$ in (3) can be chosen independent of $\nu$.

2. Integral representations

Our error analysis relies on the Laplace transform

$$\hat{u}(z) = \mathcal{L}\{u(t)\} = \int_0^\infty e^{-zt} u(t) \, dt.$$ 

A standard energy argument [11, 13] shows that $\|u(t)\| \leq \|u_0\|$ so $\hat{u}(z)$ exists and is analytic in the right half-plane $\Re z > 0$, and since $\mathcal{L}\{\partial_t^{-\nu} u\} = z^{1-\nu} \hat{u}(z)$ and $\mathcal{L}\{\partial_t u\} = z \hat{u} - u_0$, it follows from (12) that $z \hat{u}_m + \lambda_m z^{1-\nu} \hat{u}_m = u_0 m$, so

$$\hat{u}_m(z) = \frac{u_0 m}{z + \lambda_m z^{1-\nu}}.$$ 

Thus, the Laplace inversion formula gives, for $n \geq 1$ and any $a > 0$,

$$u_m(t_n) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} e^{zt} \hat{u}_m(z) \, dz = \frac{u_0 m}{2\pi i} \int_{a-i\infty}^{a+i\infty} \frac{e^{zt}}{1 + \lambda_m z^{-\nu}} \, dz,$$

which, following a substitution, we may write as

$$u_m(t_n) = \frac{u_0 m}{2\pi i} \int_{a-i\infty}^{a+i\infty} \frac{e^{nz}}{1 + \mu z^{-\nu}} \, dz \quad \text{where} \quad \mu = \lambda_m \Delta t^\nu. \quad (14)$$

It follows using Jordan’s lemma that

$$u_m(t_n) = \frac{u_0 m}{2\pi i} \int_{-\infty}^{0+} \frac{e^{nz}}{1 + \mu z^{-\nu}} \, dz \quad \text{for} \quad n \geq 1, \quad (15)$$

where the notation $\int_{-\infty}^{0^+}$ indicates that the path of integration is a Hankel contour enclosing the negative real axis and oriented counterclockwise.

Now consider the recurrence relation (6) used to compute the numerical solution. The Fourier coefficients $U_m^n = \langle U_n^t, \phi_m \rangle$ satisfy

$$(1 + \beta_0 \Delta t^\nu \lambda_m) U_m^n = U_m^{n-1} - \lambda_m \Delta t^\nu \sum_{j=1}^{n-1} \beta_{n-j} U_m^j, \quad (16)$$
and to obtain an integral representation of $U^n_m$ analogous to (15) we introduce the discrete-time Laplace transform

$$\tilde{U}(z) = \sum_{n=0}^{\infty} U^n e^{-nz}. \quad (17)$$

Again, a standard energy argument shows that $\|U^n\| \leq \|u_0\|$ so this series converges in the right half-plane $\Re z > 0$. Multiplying (16) by $e^{-nz}$, summing over $n$ and using the fact that the sum in (16) is a discrete convolution, we find that

$$[1 - e^{-z} + \mu \tilde{\beta}(z)]\tilde{U}_m(z) = [1 + \mu \tilde{\beta}(z)]u_{0m},$$

again with $\mu = \lambda_m \Delta t^\nu$. So, letting $\psi(z) = \tilde{\beta}(z)/(1 - e^{-z}),$

$$\tilde{U}_m(z) = u_{0m} \frac{1 + \mu \tilde{\beta}(z)}{1 - e^{-z} + \mu \beta(z)} = u_{0m} \frac{(1 - e^{-z})^{-1} + \mu \psi(z)}{1 + \mu \psi(z)}. \quad (18)$$

For our subsequent analysis we now establish key properties of the function $\psi(z)$.

Following appropriate shifts of the summation index, one finds that

$$\tilde{\beta}(z) = \sum_{n=0}^{\infty} \beta_n e^{-nz} = (e^z - 1)(1 - e^{-z}) \frac{\text{Li}_{-\nu}(e^{-z})}{\Gamma(1 + \nu)}, \quad (19)$$

where the polylogarithm [9, 19] is defined by $\text{Li}_p(z) = \sum_{n=1}^{\infty} z^n/n^p$ for $|z| < 1$ and $p \in \mathbb{C}$; thus,

$$\psi(z) = (e^z - 1) \frac{\text{Li}_{-\nu}(e^{-z})}{\Gamma(1 + \nu)} = \frac{1}{\Gamma(1 + \nu)} \left(1 + \sum_{n=1}^{\infty} [(n + 1)^\nu - n^\nu] e^{-nz}\right). \quad (20)$$

From the identity

$$\frac{1}{n^p} = \frac{\Gamma(1 - p)}{2\pi i} \int_{-\infty}^{\infty} e^{nw} w^{p-1} \, dw,$$

we find, after interchanging the sum and integral, that

$$\text{Li}_p(e^{-z}) = \frac{\Gamma(1 - p)}{2\pi i} \int_{-\infty}^{\infty} \frac{w^{p-1} \, dw}{e^{z-w} - 1} \quad (21)$$

for $\Re z$ sufficiently large. Thus, $\text{Li}_p(e^{-z})$ possesses an analytic continuation to the strip $-2\pi < \Im z < 2\pi$ with a cut along the negative real axis $(-\infty, 0]$. It follows that $\psi(z)$ is analytic for $z$ in the same cut strip, and moreover

$$\bar{\psi}(z) = \psi(z) \quad \text{and} \quad \psi(z + 2\pi i) = \psi(z). \quad (22)$$

**Lemma 1.** If $|\Im z| \leq \pi$ and $z \notin (-\infty, 0]$, then

$$\psi(z) = \frac{\sin \pi \nu}{\pi} \int_{0}^{\infty} \frac{e^{-s} - 1 - e^{-z-s}}{1 - e^{-z-s}} \frac{1 - e^{-s}}{s} \, ds \quad (23)$$

and $1 + \mu \psi(z) \neq 0$ for $0 < \mu < \infty$. 

6
Proof. Given \( z \notin (-\infty, 0] \), we can choose a Hankel contour that does not enclose \( z \), and the formulae (20) and (21) then imply that

\[
\psi(z) = e^{z - 1} \frac{1}{2\pi i} \int_{-\infty}^{0+} \frac{w^{-\nu-1}}{e^z - w^\nu} \, dw.
\]

Since

\[
\frac{e^z - 1}{e^z - w^\nu} = 1 + \frac{e^w - 1}{1 - e^{w-z}} \quad \text{and} \quad \int_{-\infty}^{0+} w^{-\nu-1} \, dw = 0,
\]

we have

\[
\psi(z) = \frac{1}{2\pi i} \int_{-\infty}^{0+} \frac{w^{-\nu}}{1 - e^{w-z}} \frac{e^w - 1}{w} \, dw.
\]

Define contours along either side of the cut,

\[
C_\pm = \{ se^{\pm i\pi} : 0 < s < \infty \},
\]

so that \( \arg(w) = \pm \pi \) if \( w \in C_\pm \). Noting that the integrand is \( O(w^{-\nu}) \) as \( w \to 0 \), we may collapse the Hankel contour into \( C^- - C^+ \) to obtain (23).

The second part of the lemma amounts to showing that \( \psi(z) \notin (-\infty, 0] \). If \( x \geq 0 \) and \( \alpha_n = e^{-x^n} [(n+1)^\nu - n^\nu] \), then

\[
\psi(x + iy) = \frac{1}{\Gamma(1+\nu)} \left( 1 + \sum_{n=1}^{\infty} \alpha_n \cos ny - i \sum_{n=1}^{\infty} \alpha_n \sin ny \right).
\]

The sequence \( \alpha_n \) is convex and tends to zero, so [21 pp. 183 and 228]

\[
\Re \psi(x + iy) \geq \frac{1}{2\Gamma(1+\nu)} \quad \text{and} \quad \Im \psi(x + iy) < 0 \quad \text{for} \ x \geq 0 \ \text{and} \ 0 < y < \pi,
\]

and using [22] we find that \( \Im \psi(x \pm i\pi) = 0 \) for \( -\infty < x < \infty \). The polylogarithm satisfies [19 Equation (3.1)]

\[
\Im \text{Li}_p(e^{-z}) = -\frac{\pi^p s^{p-1}}{\Gamma(p)} \quad \text{if} \quad z = se^{\pm i\pi} \quad \text{for} \ 0 < s < \infty,
\]

so, using the identity \( \Gamma(1+\nu)\Gamma(1-\nu) = \pi \nu/\sin \pi \nu \),

\[
\Im \psi(se^{\pm i\pi}) = \mp (1 - e^{-s}) s^{-\nu-1} \sin \pi \nu,
\]

and in particular \( \Im \psi(x + i0) < 0 \) but \( \Im \psi(x - i0) > 0 \) for \( -\infty < x < 0 \), whereas \( \Im \psi(x) = 0 \) for \( 0 < x < \infty \). Applying the strong maximum principle for harmonic functions, we conclude that \( \Im \psi(x + iy) \neq 0 \) if \( 0 < |y| < \pi \). We saw above that \( \Re \psi(x + iy) > 0 \) if \( x \geq 0 \), and by (23),

\[
\psi(x \pm i\pi) = \frac{\sin \pi \nu}{\pi} \int_{0}^{\infty} \frac{s^{-\nu-1} - e^{-s}}{1 + e^{-x-s}} \, ds > 0
\]

for all real \( x \), which completes the proof. \( \square \)
Since
\[
\frac{1}{2\pi i} \int_{a-i\pi}^{a+i\pi} e^{(n-j)z} \, dz = \delta_{nj} = \begin{cases} 1, & \text{if } n = j, \\ 0, & \text{if } n \neq j, \end{cases}
\]
we see from the definition (17) of \(\tilde{U}_m\), after interchanging the sum and integral, that for any \(a > 0\),
\[
U_n^m = \frac{1}{2\pi i} \int_{a-i\pi}^{a+i\pi} e^{nz} \tilde{U}_m(z) \, dz.
\]
Moreover, since
\[
\frac{(1 - e^{-z})^{-1} + \mu \psi(z)}{1 + \mu \psi(z)} = 1 + \frac{(1 - e^{-z})^{-1} - 1}{1 + \mu \psi(z)} = 1 - \frac{1/(1 - e^z)}{1 + \mu \psi(z)},
\]
the formula (18) for \(\tilde{U}_m(z)\) implies that
\[
U_n^m = \frac{u_{0m}}{2\pi i} \int_{a-i\pi}^{a+i\pi} \frac{e^{nz}}{1 + \mu \psi(z)} \frac{dz}{e^z - 1} \quad \text{for } n \geq 1.
\]

The next lemma describes the asymptotic behaviour of \(\psi\), and shows in particular that the integrands of (14) and (28) are close for \(z\) near 0. In (29), \(\zeta\) denotes the Riemann zeta function.

**Lemma 2.** The function (20) satisfies
\[
\psi(z) = z^{-\nu} + \frac{1}{2} z^{1-\nu} + \frac{\zeta(-\nu)}{\Gamma(1 + \nu)} z + O(z^{2-\nu}) \quad \text{as } z \to 0,
\]
and
\[
\psi(z) = \frac{\sin \pi \nu}{\pi \nu} (i\pi - z)^{-\nu} + O(z^{-\nu-1}) \quad \text{as } \Re(z) \to -\infty, \text{ with } 0 < \Im z < \pi.
\]

**Proof.** Flajolet [4, Theorem 1] shows that
\[
\text{Li}_p(e^{-z}) \sim (1-p)z^{p-1} + \sum_{k=0}^{\infty} (-1)^k \zeta(p-k) \frac{z^k}{k!} \quad \text{as } z \to 0,
\]
and (29) follows because \(e^z - 1 = z + \frac{1}{2} z^2 + O(z^3)\) as \(z \to 0\). The results of Ford [14, Equation (17), p. 226] imply that
\[
\text{Li}_p(e^{-z}) = -\frac{(i\pi - z)^p}{\Gamma(1 + p)} + O(z^{p-1}) \quad \text{as } \Re z \to -\infty,
\]
(see also Wood [19, Equation (11.2)]) which, in combination with the identity \(\Gamma(1 + \nu)\Gamma(1 - \nu) = \pi \nu / \sin \pi \nu\), implies (30).

The formula for \(U_n^m\) in the next theorem matches (15) for \(u_m(t_n)\).
Figure 1: The integration contour $C(a,M)$.

**Theorem 3.** The solution of (16) admits the integral representation

$$U_n^m = u_0 \frac{1}{2\pi i} \int_{-\infty}^{0^+} e^{nx} \frac{dz}{1 + \mu \psi(z)} \frac{1}{e^z - 1}$$

for $n \geq 1$, (33)

where the Hankel contour remains inside the strip $-\pi < \Im z < \pi$.

**Proof.** By Lemma 1, the integrand from (28) is analytic for $z$ inside the contour $C(a,M)$ shown in Figure 1. The contributions along $\Im z = \pm \pi$ cancel in view of the second part of (22). Using (30), if $\Re z \to -\infty$ then

$$\frac{1}{e^z - 1} \sim (1 + \mu \sin \frac{\pi \nu}{\pi \nu} (i\pi - z)^{-\nu})^{-1} \sim -1 + \mu \frac{\sin \pi \nu}{\pi \nu} (i\pi - z)^{-\nu},$$

so the contributions along $\Re z = -M$ are $O(e^{-nM})$ as $M \to \infty$, implying the desired formula for $U_n^m$.

Together, (15) and (33) imply that the error formula (13) holds, with

$$\delta_n^a(\mu) = \frac{1}{2\pi i} \int_{-\infty}^{0^+} e^{nx} \left( \frac{1}{1 + \mu \psi(z)} \frac{z}{e^z - 1} - \frac{1}{1 + \mu z^{-\nu}} \right) \frac{dz}{z}$$

for $0 < \mu < \infty$, and with $\delta_n^a(0) = 0$ because if $\lambda_m = 0$ then $u_m(t_n) = u_0 = U_m^n$ for all $n$. The following estimate for $\delta_n^a(\mu)$ is the key to proving our error estimates, but the lengthy proof is deferred until Section 4.

**Theorem 4.** Let $0 < \nu < 1$. The sequence (34) satisfies

$$|\delta_n^a(\mu)| \leq C n^{-1} \min((\mu n^\nu)^2, (\mu n^\nu)^{-1})$$

for $n = 1, 2, 3, \ldots$ and $0 < \mu < \infty$.

**Proof.** Follows from Theorems 12 and 16.

9
We remark that in the limiting case $\nu \to 1$, when our method reduces to the classical implicit Euler scheme (8) for the heat equation (7), it is readily seen that the error representation (13) holds with $\delta^n(\mu) = (1 + \mu)^{-n} - e^{-n\mu}$, and that $0 \leq \delta^n(\mu) \leq Cn^{-1} \min((\mu)2, (\mu)n^{-1})$, consistent with Theorem 4.

3. Error estimates

We begin this section with the basic error bound that applies even when no smoothness is assumed for the initial data.

**Theorem 5.** For any $u_0 \in H$, the solutions of (1) and (5) satisfy

$$
\|U^n - u(t_n)\| \leq Ct_n^{1-\nu} \|u_0\| \quad \text{for } n = 1, 2, 3, \ldots
$$

**Proof.** Theorem 4 implies that $|\delta^n(\mu)| \leq Cn^{-1}$ uniformly for $0 < \mu < \infty$, and since the $\phi_m$ are orthonormal, we see from (13) that

$$
\|U^n - u(t_n)\|^2 = \sum_{m=1}^{\infty} \left[\delta^n(\lambda_m t^{\nu}) u_{0m}\right]^2 \leq (Cn^{-1})^2 \sum_{m=1}^{\infty} u_{0m}^2 = (Cn^{-1} \|u_0\|)^2.
$$

The estimate follows after recalling that $t_n = n \Delta t$ so $n^{-1} = t_n^{-1} \Delta t$.

For smoother initial data, the error bound exhibits a less severe deterioration as $t_n$ approaches zero.

**Lemma 6.** Consider the solutions of (1) and (5).

1. If $0 < \nu \leq 1/2$ and $A^2 u_0 \in H$, then

$$
\|U^n - u(t_n)\| \leq Ct_n^{2\nu-1} \|A^2 u_0\| \leq C \Delta t^{2\nu} \|A^2 u_0\|.
$$

2. If $1/2 < \nu < 1$ and $A^{1/\nu} u_0 \in H$, then

$$
\|U^n - u(t_n)\| \leq C \Delta t \|A^{1/\nu} u_0\|.
$$

**Proof.** In the first case, since $\lambda_m \Delta t^{\nu} = \lambda_m t^{\nu}_n$,

$$
|\delta^n(\lambda_m \Delta t^{\nu})| \leq Ct_n^{-1} \Delta t \min((\lambda_m t^{\nu}_n)^2, (\lambda_m t^{\nu}_n)^{-1})
$$

$$
= Ct_n^{2\nu-1} \Delta t \lambda_m^2 \min(1, (\lambda_m t^{\nu}_n)^{-3}) \leq Ct_n^{2\nu-1} \Delta t \lambda_m^2,
$$

so by (10) and (35),

$$
\|U^n - u(t_n)\|^2 \leq \sum_{m=1}^{\infty} \left(Ct_n^{2\nu-1} \Delta t \lambda_m^2 u_{0m}\right)^2 = \left(Ct_n^{2\nu-1} \Delta t \|A^2 u_0\|\right)^2,
$$

with $t_n^{2\nu-1} \Delta t = n^{2\nu-1} \Delta t^{2\nu} \leq \Delta t^{2\nu}$. The second case follows in a similar fashion, because $n^{-1} = \Delta t \lambda_m^{1/\nu} (\lambda_m t^{\nu}_n)^{-1/\nu}$ implies that

$$
|\delta^n(\lambda_m \Delta t^{\nu})| \leq C \Delta t \lambda_m^{1/\nu} \min((\lambda_m t^{\nu}_n)^{-2-1/\nu}, (\lambda_m t^{\nu}_n)^{-1-1/\nu}) \leq C \Delta t \lambda_m^{1/\nu}.
$$
We are now ready to prove our main result.

**Theorem 7.** The solutions of (1) and (5) satisfy
\[
\|U_n - u(t_n)\| \leq C t_r^{\nu - 1} \Delta t \|A^r u_0\| \quad \text{for } 0 \leq r \leq \min(2, 1/\nu).
\]

**Proof.** If \(0 < \nu \leq 1/2\) and \(0 < \theta < 1\), then by interpolation
\[
\|U_n - u(t_n)\| \leq C (t_r^{-1} \Delta t)^{1-\theta} (t_n^{2r-1} \Delta t) \|A^{2r} u_0\| = C t_r^{2r-1} \Delta t \|A^{2r} u_0\|,
\]
and the estimate follows by putting \(r = 2\). Similarly, if \(1/2 \leq \nu < 1\), then
\[
\|U_n - u(t_n)\| \leq C (t_r^{-1} \Delta t)^{1-\theta} \Delta t^{\theta} \|A^{\theta/r} u_0\| = C t_r^{\theta - 1} \Delta t \|A^{\theta/r} u_0\|,
\]
and the estimate follows by putting \(r = \theta/\nu\). \(\square\)

4. Technical proofs

It remains to prove Theorem 4. In this section only, \(C\) always denotes an absolute constant and we use subscripts in cases where the constant might depend on some parameters; for instance \(C_{\nu}\) may depend on the fractional diffusion exponent \(\nu\).

Since the integrand of (34) is \(O(z^{\nu - 1})\) as \(z \to 0\), we may collapse the Hankel contour onto \(C_+ - C_-\) for \(C_{\pm}\) given by (24). In this way, defining
\[
\psi_{\pm}(s) = \psi(se^{\pm i\pi}) \quad \text{for } 0 < s < \infty,
\]
we find that
\[
\int_{C_{\pm}} e^{nz} \left( \frac{1}{1 + \mu \psi(z)} \frac{z}{e^z - 1} - \frac{1}{1 + \mu z^{-\nu}} \right) \frac{dz}{z} = \int_0^\infty e^{-ns} \left( \frac{1}{1 + \mu \psi_{\pm}(s)} \frac{s}{1 - e^{-s}} - \frac{1}{1 + \mu s^{-\nu} e^{\mp i\pi \nu}} \right) \frac{ds}{s}.
\]
By (22) and (26),
\[
\psi_-(s) = \psi_+(s) \quad \text{and} \quad \Im \psi_{\pm}(s) = \pm (1 - e^{-s}) s^{-\nu - 1} \sin \pi \nu,
\]
so
\[
\frac{1}{1 + \mu \psi_+(s)} - \frac{1}{1 + \mu \psi_-(s)} = \frac{2i\mu \Im \psi_-(s)}{|1 + \mu \psi_+(s)|^2} = \frac{2i\mu s^{-\nu} \sin \pi \nu}{|1 + \mu \psi_+(s)|^2} \frac{1 - e^{-s}}{s},
\]
and similarly,
\[
\frac{1}{1 + \mu s^{-\nu} e^{-i\pi \nu}} - \frac{1}{1 + \mu s^{-\nu} e^{i\pi \nu}} = \frac{2i\mu s^{-\nu} \sin \pi \nu}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2}.
\]
Thus, the representation (34) implies
\[
\delta_n(\mu) = \frac{\sin \pi \nu}{\pi} \int_0^\infty e^{-ns} \mu s^{-\nu} \left( \frac{1}{|1 + \mu \psi_+(s)|^2} - \frac{1}{|1 + \mu s^{-\nu} e^{-i\pi \nu}|^2} \right) \frac{ds}{s}.
\]
We will estimate this integral with the help of the following sequence of lemmas.
Lemma 8. If $X \geq 0$ then $|1 + X e^{\pm i \nu}|^{-2} \leq (1 - \nu)^{-2}(1 + X^2)^{-1}$.

Proof. Since $0 \leq 2X/(1 + X^2) \leq 1$,
\[
\frac{|1 + X e^{\pm i \nu}|^2}{1 + X^2} = \frac{|e^{\mp i \nu} + X|^2}{1 + X^2} = 1 + \frac{2X}{1 + X^2} \cos \pi \nu \geq \min(1, 1 + \cos \pi \nu),
\]
and the result follows because $1 + \cos \pi \nu = 2\cos^2(\pi \nu/2) \geq 2(1 - \nu)^2$. \hfill \square

Lemma 9. If $\mu \geq 0$ and $s > 0$, then $|1 + \mu \psi_{\pm}(s)|^{-2} \leq C_\nu(1 + \mu^2 s^{-2\nu})^{-1}$.

Proof. Lemma 2 implies that
\[
\psi_{\pm}(s) = e^{\mp i \nu}(s^{-\nu} - \frac{1}{2}s^{-1-\nu}) - \frac{\zeta_{\pm}(s)}{\Gamma(1 + \nu)} s + O(s^{2-\nu}) \quad \text{as } s \to 0 \quad (38)
\]
and
\[
\psi_{\pm}(s) = \frac{\sin \pi \nu}{\pi \nu} s^{-\nu} + O(s^{-\nu-1}) \quad \text{as } s \to \infty. \quad (39)
\]
Thus, if we define $\phi(s) = s^\nu \psi_{\pm}(s)$ for $0 < s < \infty$, with
\[
\phi(0) = e^{-i \pi \nu} \quad \text{and} \quad \phi(\infty) = \frac{\sin \pi \nu}{\pi \nu}, \quad (40)
\]
then $\phi$ is continuous on the one-point compactification $[0, \infty]$ of the closed half-line $[0, \infty)$. Put $X = \mu s^{-\nu}$ and define
\[
f(s, X) = \frac{|1 + \mu \psi_{\pm}(s)|^2}{1 + X^2} = \frac{|1 + X \phi(s)|^2}{1 + X^2}
\]
for $0 \leq s \leq \infty$ and $0 \leq X < \infty$, with $f(s, \infty) = |\phi(s)|^2$, so that $f$ is continuous on the compact topological space $[0, \infty] \times [0, \infty)$. It therefore suffices to prove that $f$ is strictly positive everywhere. By (36),
\[
\Im \phi(s) = -\frac{1 - e^{-s}}{s} \sin \pi \nu < 0 \quad \text{for } 0 < s < \infty, \quad (41)
\]
and $\Im \phi(0) = -\sin \pi \nu < 0$ by (40), so $|1 + X \phi(s)|^2 \geq |X \Im \phi(s)|^2 > 0$ for $0 \leq s < \infty$ and $0 < X < \infty$. Moreover, $|1 + X \phi(\infty)|^2 \geq 1$ because $\phi(\infty)$ is real and positive, and $f(s, 0) = 1$ for $0 \leq s \leq \infty$. Finally, (40) and (41) imply that $f(s, \infty) = |\phi(s)|^2 > 0$ for $0 \leq s \leq \infty$. \hfill \square

Lemma 10. For $\mu \geq 0$ and $s > 0$,
\[
|1 + \mu s^{-\nu} e^{\mp i \pi \nu}|^{-2} - |1 + \mu \psi_{\pm}(s)|^2
\]
\[
= \mu B_+(s)(1 + \mu s^{-\nu} e^{\mp i \pi \nu}) + \mu B_-(s)(1 + \mu \psi_{\pm}(s)) = \mu B_1(s) + \mu^2 B_2(s),
\]
where $B_{\pm}(s) = s^{-\nu} e^{\mp i \pi \nu} - \psi_{\pm}(s)$ and
\[
B_1(s) = B_+(s) + B_-(s) = 2(s^{-\nu} \cos \pi \nu - \Re \psi_{\pm}(s)),
\]
\[
B_2(s) = B_+(s)s^{-\nu} e^{i \pi \nu} + B_-(s)\psi_+(s) = s^{-2\nu} - \psi_+(s)\psi_-(s).
\]
Proof. Put \( a = \mu s^{-\nu} e^{-i\pi \nu} \) and \( b = \mu \psi \pm \) in the identities

\[
|1 + a|^2 - |1 + b|^2 = (a - b)(1 + \bar{a} + \bar{b})(1 + b)
= (a - b) + (\bar{a} - \bar{b}) + (a\bar{a} - b\bar{b}).
\]

Notice that \( B_1 \) and \( B_2 \) are real, whereas \( B_\pm(s) = \overline{B_\pm(s)} \).

Lemma 11. As \( s \to 0 \),

\[
B_\pm(s) = O(s^{1-\nu}), \quad B_1(s) = s^{1-\nu} \cos \pi \nu + O(s), \quad B_2(s) = s^{1-2\nu} + O(s^{1-\nu}),
\]
and as \( s \to \infty \),

\[
B_\pm(s) = O(s^{-\nu}), \quad B_1(s) = O(s^{-\nu}), \quad B_2(s) = O(s^{-2\nu}).
\]

Proof. Follows using (38) and (39).

We are now ready to prove the easier half of Theorem 4.

Theorem 12. For \( 0 < \mu < \infty \) and \( n = 1, 2, 3, \ldots \), the sequence (34) satisfies

\[
|\delta_n(\mu)| \leq C \nu n^{-1} \rho^{-1} \quad \text{if} \quad \rho = \mu \nu.
\]

Proof. From (37) and Lemma 10, we see that

\[
\frac{\sin \pi \nu}{\pi} \int_0^\infty e^{-ns} \mu s^{-\nu} \mu B_+(s) \left( 1 + \mu s^{-\nu} e^{i\pi \nu} \right) \mu B_-(s) \left( 1 + \mu \psi_+(s) \right) \frac{ds}{s},
\]
and thus, by Lemmas 8 and 13

\[
|\delta_n(\mu)| \leq C \nu \int_0^\infty e^{-ns} \mu s^{-\nu} \frac{\mu |B_\pm(s)|}{(1 + \mu^2 s^{-2\nu})^{3/2}} \frac{ds}{s}.
\]

Lemma 11 implies that \( |B_\pm(s)| \leq C \nu \min(s^{1-\nu}, s^{-\nu}) = C \nu s^{-\nu} \min(s, 1) \), so

\[
|\delta_n(\mu)| \leq C \nu \int_0^\infty g_n(s, \mu) ds \quad \text{where} \quad g_n(s, \mu) = e^{-ns} \mu^2 s^{-2
-1} \min(s, 1) \frac{(1 + \mu^2 s^{-2\nu})^{3/2}}{n \rho}.
\]

The estimate for \( \delta_n(\mu) \) follows because

\[
\int_0^1 g_n(s, \mu) ds \leq \int_0^1 e^{-ns} \frac{s^{\nu}}{\mu} ds = \frac{n^{1-\nu}}{\mu} \int_0^n e^{-s} s^{\nu} ds \leq \frac{\Gamma(1 + \nu)}{n \rho}
\]
and

\[
\int_1^\infty g_n(s, \mu) ds \leq \int_1^\infty e^{-ns} \frac{s^{\nu-1}}{\mu} ds \leq \int_1^\infty \frac{e^{s}}{\mu} ds = \frac{n^\nu}{\rho} \leq \frac{C}{n \rho}.
\]
Establishing the behaviour of $\delta^n(\mu)$ when $\rho = \mu \nu^\nu$ is small turns out to be more delicate, and relies on three additional lemmas.

**Lemma 13.** If $0 \leq \nu \leq 1/2$ then $x^\nu \int_x^1 s^{-3\nu} \, ds \leq 3$ for $0 < x \leq 1$.

**Proof.** Let $f(x) = x^\nu \int_x^1 s^{-3\nu} \, ds$. If $0 < \nu < 1/3$ then

$$f'(x) > 0 \text{ for } 0 < x < x^* \quad \text{and} \quad f'(x) < 0 \text{ for } x^* < x < 1,$$

where $x^* = [\nu/(1 - 2\nu)]^{1/(1-3\nu)} < 1$. Since $f'(x) = \nu x^{-1} f(x) - x^{-2\nu},$

$$f(x) \leq f(x^*) = \frac{(x^*)^{1-2\nu}}{\nu} = \frac{(x^*)^{\nu}}{1-2\nu} \leq 3.$$ If $\nu = 1/3$, then $f(x) = x^{1/3} \log x^{-1}$ and (42) holds with $x^* = e^{-3}$, implying that $f(x) \leq f(x^*) = 3e^{-1} \leq 3$. If $1/3 < \nu < 1/2$, then (42) holds with $x^* = [(1 - 2\nu)/\nu]^{1/(3\nu-1)} < 1$ and again $f(x) \leq f(x^*) = (x^*)^{1-2\nu}/\nu \leq 3$. Finally, if $\nu = 0$ then $f(x) = 1 - x \leq 1$, and if $\nu = 1/2$ then $f(x) = 2(1 - x^{1/2}) \leq 2$. 

**Lemma 14.** If $1/2 \leq \nu \leq 1$ then $x^{\nu-1} \int_1^x s^{1-3\nu} \, ds \leq 3$ for $1 \leq x < \infty$.

**Proof.** Make the substitutions $x' = x^{-1}, s' = s^{-1}, \nu' = 1 - \nu$ in Lemma 13.

**Lemma 15.** If $1/2 < \nu < 1$ then

$$\int_0^\infty \frac{s^{-2\nu} \cos \pi \nu + s^{-3\nu}}{|1 + s^{-\nu} e^{i\pi \nu}|^4} \, ds = \int_0^\infty \frac{s^{\nu} + s^{2\nu} \cos \pi \nu}{|s^{\nu} + e^{i\pi \nu}|^4} \, ds = 0.$$
Proof. Let \( p = -\cos \pi \nu \) so that \( 0 < p < 1 \). Making the substitution \( x = s^\nu \), we see that the integral equals \( \nu^{-1} I \), where
\[
I = \int_0^\infty f(x) \, dx \quad \text{and} \quad f(x) = \frac{1 - px}{(x^2 - 2px + 1)^{\nu/2}} x^{1/\nu}.
\]
We consider the analytic continuation of \( f \) to the cut plane \( \mathbb{C} \setminus [0, \infty) \), and note that \( z^2 - 2pz + 1 = (z - \alpha_+)(z - \alpha_-) \) where \( \alpha_\pm = p \pm iq = e^{i\pi(1 \pm \nu)} \) and \( q = \sqrt{1 - p^2} = \sin \pi \nu \). Thus, \( f \) has double poles at \( z = \alpha_+ \) and at \( \alpha_- \). Moreover, since \( 1 < 1/\nu < 2 \) we see that \( f(z) = \mathcal{O}(|z|^{-1}) \) as \( |z| \to \infty \), and that \( f(z) = \mathcal{O}(|z|) \) as \( |z| \to 0 \). After integrating around the contour \( C(\epsilon, R) \) shown in Figure 2 and sending \( \epsilon \to 0^+ \) and \( R \to \infty \), we conclude that
\[
\frac{1 - e^{i2\pi/\nu}}{2\pi i} I = \text{res}_{z=\alpha_+} f(z) + \text{res}_{z=\alpha_-} f(z).
\]
Since \( (z - \alpha_\pm)^2 f(z) = (1 - pz)z^{1/\nu}/(z - \alpha_\pm)^2 \) and \( \alpha_1^{1/\nu} = -e^{i\pi/\nu} = \alpha_1^{1/\nu} \),
\[
\text{res}_{z=\alpha_\pm} f(z) = \lim_{z \to \alpha_\pm} \frac{d}{dz} (z - \alpha_\pm)^2 f(z) = \frac{d}{dz} \left[ \frac{(1 - pz)z^{1/\nu}}{(z - \alpha_\pm)^2} \right]_{z=\alpha_\pm} = \mp i \frac{1 - \nu}{\nu} \frac{e^{i\pi/\nu}}{4q},
\]
showing that the residues cancel, and therefore \( I = 0 \) because \( e^{i2\pi/\nu} \neq 1 \).

Our final result for this section completes the proof of Theorem 16 and hence of the error estimates of Section 3.

**Theorem 16.** For \( 0 < \mu < \infty \) and \( n = 1, 2, 3, \ldots \), the sequence (34) satisfies
\[
|\delta^n(\mu)| \leq C_\nu n^{-1} \rho^2 \quad \text{if} \quad \rho = \mu \nu^\nu \leq 1.
\]

**Proof.** By Lemma 11,
\[
\mu B_1(s) + \mu^2 B_2(s) = s \left( \mu s^{-\nu} \cos \pi \nu + (\mu s^{-\nu})^2 + \mathcal{O}(\mu + \mu^2 s^{-\nu}) \right) \quad \text{as} \quad s \to 0^+,
\]
and \( \mu B_1(s) + \mu^2 B_2(s) = \mathcal{O}(\mu s^{-\nu} + \mu^2 s^{-2\nu}) \) as \( s \to \infty \), so (37) implies that
\[
|\delta^n(\mu)| = \left| \frac{\sin \pi \nu}{\pi} \int_0^\infty e^{-ns} \mu s^{-\nu} \frac{\mu B_1(s) + \mu^2 B_2(s)}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2 |1 + \mu \psi(s)|^2} \, ds \right|
\leq \frac{\sin \pi \nu}{\pi} \left( |I_1| + C_\nu I_2 + C_\nu I_3 \right),
\]
where, using Lemmas 8 and 9
\[
I_1 = \int_0^1 e^{-ns} \mu s^{-\nu} \frac{\mu s^{-\nu} \cos \pi \nu + (\mu s^{-\nu})^2}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2 |1 + \mu \psi(s)|^2} \, ds,
\]
\[
I_2 = \int_0^1 e^{-ns} \mu s^{-\nu} \frac{\mu + \mu^2 s^{-\nu}}{(1 + \mu^2 s^{-2\nu})^2} \, ds, \quad I_3 = \int_1^\infty e^{-ns} \mu s^{-\nu} \frac{\mu s^{-\nu} + \mu^2 s^{-2\nu}}{(1 + \mu^2 s^{-2\nu})^2} \, ds.
\]
Put $f(x) = (x + x^2)/(1 + x^2)^2$ so that
\[
I_2 = \mu \int_0^1 e^{-ns} f(\mu s^{-\nu}) \, ds = n^{-1-\nu} \rho \int_0^n e^{-s} f(\rho s^{-\nu}) \, ds.
\]
Since $f(x) \leq \min(2x, x^{-2})$ we have $f(\rho s^{-\nu}) \leq C \min(\rho^{-2} s^{2\nu}, \rho s^{-\nu})$ and thus
\[
n^{1+\nu} \rho^{-1} I_2 \leq C \rho^{-2} \int_0^{\rho^{1/\nu}} e^{-s} s^{2\nu} \, ds + C \rho \int_{\rho^{1/\nu}}^n e^{-s} s^{-\nu} \, ds
\leq C \int_0^{\rho^{1/\nu}} e^{-s} \, ds + C \rho \int_0^1 s^{-\nu} \, ds + C \rho \int_1^\infty e^{-s} \, ds
\leq C \rho^{1/\nu} + C(1 - \nu)^{-1} \rho + C \rho \leq C(1 - \nu)^{-1} \rho + C \rho^{1/\nu} \leq C \rho,
\]
implying $I_2 \leq C \nu n^{-1-\nu} \rho^2 \leq C \nu n^{-1} \rho^2$. Noting that $\mu = \rho n^{-\nu} \leq 1$, we have
\[
I_3 \leq \int_1^{\infty} e^{-ns} \mu^2 s^{-2\nu-1} \, ds \leq \mu^2 \int_1^{\infty} e^{-ns} \, ds = \mu^2 e^{-n} \leq n^{-1} \mu^2 = n^{-1-2\nu} \rho^2,
\]
and therefore $I_3 \leq n^{-1} \rho^2$.

It remains to estimate $I_1$. First consider the case $0 < \nu < 1/2$, in which $\cos \pi \nu > 0$. Put $g(x) = (x^2 \cos \pi \nu + x^3)/(1 + x^2)^2$, so that
\[
I_1 \leq C \nu \int_0^1 e^{-ns} g(\mu s^{-\nu}) \, ds = C \nu n^{-1} \int_0^n e^{-s} g(\rho s^{-\nu}) \, ds.
\]
Since $g(x) \leq \min(2x^2, x^{-2} \cos \pi \nu + x^{-1})$ we have
\[
g(\rho s^{-\nu}) \leq C \min(\rho^{-1} s^{\nu}, \rho^2 s^{-2\nu} \cos \pi \nu + \rho^3 s^{-3\nu})
\]
and hence $\int_0^n e^{-s} g(\rho s^{-\nu}) \, ds$ is bounded by
\[
C \rho^{-1} \int_0^{\rho^{1/\nu}} s^{\nu} \, ds + C \rho^2 \cos \pi \nu \int_0^n e^{-s} s^{-2\nu} \, ds + C \rho^3 \int_0^n e^{-s} s^{-3\nu} \, ds
\leq C \rho^{1/\nu} + C \rho^2 \int_0^1 (1 - 2\nu) s^{-2\nu} \, ds + C \rho^3 \int_1^{\infty} s^{-3\nu} \, ds + C \rho^2 \int_1^{\infty} e^{-s} \, ds.
\]
Applying Lemma 13 with $x = \rho^{1/\nu}$ and noting that $1/\nu > 2$, it follows that
\[
\int_0^n e^{-s} g(\rho s^{-\nu}) \, ds \leq C \left( \rho^{1/\nu} + \rho^2 \right)
\]
and hence $I_1 \leq C \nu n^{-1} \rho^2$.

If $\nu = 1/2$, then $\cos \pi \nu = 0$ and the argument above again shows that $I_1 \leq C \nu n^{-1} \rho^2$. Thus, assume now that $1/2 < \nu < 1$ and note $\cos \pi \nu < 0$. Since
\[
\frac{e^{-ns}}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2} \frac{1}{|1 + \mu^2 s^{-\nu} e^{i\pi \nu}|^2} = \frac{1}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2}
\]
and noting that $1/n > 2$, it follows that
\[
\int_0^n e^{-s} g(\rho s^{-\nu}) \, ds \leq C \left( \rho^{1/\nu} + \rho^2 \right)
\]
and hence $I_1 \leq C \nu n^{-1} \rho^2$.
and, by Lemma 15,

$$
\int_{0}^{1} \frac{(\mu s - \nu)^2 \cos \pi \nu + (\mu s - \nu)^3}{|1 + \mu s e^{i \pi \nu}|^4} \, ds = \mu^{1/\nu} \int_{0}^{\rho^{1/\nu}} \frac{s^{-2\nu} \cos \pi \nu + s^{-3\nu}}{|1 + s^{-\nu} e^{i \pi \nu}|^4} \, ds
$$

$$
= -\mu^{1/\nu} \int_{\rho^{1/\nu}}^{\infty} \frac{s^{-2\nu} \cos \pi \nu + s^{-3\nu}}{|1 + s^{-\nu} e^{i \pi \nu}|^4} \, ds,
$$

we have

$$
|I_1| \leq C_\nu (J_1 + J_2 + J_3),
$$

where

$$
J_1 = \mu^{1/\nu} \int_{\rho^{1/\nu}}^{\infty} \frac{s^{-2\nu} \cos \pi \nu + s^{-3\nu}}{(1 + \mu^2 s^{-\nu})^2} \, ds,
$$

$$
J_2 = \int_{0}^{1} (1 - e^{-ns}) \frac{(\mu s - \nu)^2 |\cos \pi \nu| + (\mu s - \nu)^3}{(1 + \mu^2 s^{-\nu})^2} \, ds,
$$

$$
J_3 = \int_{0}^{1} \frac{[(1 + \mu s^0 e^{i \pi \nu})^2 - |1 + \mu \psi_+ (s)|^2]}{(1 + \mu^2 s^{-\nu})^2} \, ds.
$$

First, because $\mu^{1/\nu} = n^{-1} \rho^{1/\nu}$ and $|\cos \pi \nu| = \sin \pi (\nu - \frac{1}{2}) \leq \pi (\nu - \frac{1}{2})$,

$$
J_1 \leq C n^{-1} \rho^{1/\nu} \int_{n \rho^{1/\nu}}^{\infty} ((2\nu - 1)s^{-2\nu} + s^{-3\nu}) \, ds
$$

$$
\leq C n^{-1} \rho^{1/\nu} [(n \rho^{-1/\nu})^{1-2\nu} + (n \rho^{-1/\nu})^{1-3\nu}]
$$

$$
= C n^{-2\nu} \rho^2 + C n^{-3\nu} \rho^3 \leq C n^{-1} \rho^2.
$$

Second, since $1 - e^{-x} \leq x$ and $\mu^{1/\nu} = n \rho^{-1/\nu} \geq 1$, we see that $n \rho^{-1/\nu} J_2$ equals

$$
\int_{0}^{n \rho^{-1/\nu}} (1 - e^{-\rho^{1/\nu} s}) \frac{s^{-2\nu} |\cos \pi \nu| + s^{-3\nu}}{(1 + s^{-\nu})^2} \, ds \leq C \int_{0}^{1} (1 - e^{-\rho^{1/\nu} s}) s^{-3\nu} \, ds
$$

$$
+ C \int_{1}^{n \rho^{-1/\nu}} (1 - e^{-\rho^{1/\nu} s}) (s^{-2\nu} (\nu - \frac{1}{2}) + s^{-3\nu}) \, ds
$$

$$
\leq C \rho^{1/\nu} \int_{0}^{1} s^{\nu+1} \, ds + C \int_{\rho^{1/\nu}}^{n} (1 - e^{-s}) (\rho^3 s^{-3\nu} + (\nu - \frac{1}{2}) \rho^2 s^{-2\nu}) \, ds.
$$

Since $\rho^3 s^{-3\nu} \leq \rho^2 s^{-2\nu}$ for $s \geq \rho^{1/\nu}$, the last integral is bounded by

$$
\int_{\rho^{1/\nu}}^{1} 2\rho^{2} s^{1-2\nu} \, ds + C \int_{1}^{n} (2\nu - 1) (\rho^3 s^{-3\nu} + \rho^2 s^{-2\nu}) \, ds
$$

$$
\leq C \int_{\rho^{1/\nu}}^{1} \rho^{2} s^{-1} \, ds + C \rho^3 + C \rho^2 \leq C \rho^{3-1/\nu} + C \rho^2 \log \rho^{-1/\nu},
$$

and thus

$$
J_2 \leq C n^{-1} \rho^{1/\nu} (\rho^{1/\nu} + C \rho^{3-1/\nu} + \nu^{-1} \rho^2 \log \rho^{-1}) \leq C n^{-1} \rho^2.
$$
Third, by Lemmas 10 and 11,

\[ J_3 \leq \int_0^1 (\mu s^{1-\nu} + \mu^2 s^{1-2\nu}) \frac{\mu s^{-\nu}}{(1 + \mu s^{-\nu})^3} ds \]

\[ = \mu^{1+1/\nu} \int_0^{\nu^{-1/\nu}} \frac{s(s^{-\nu} + s^{-2\nu})(s^{-2\nu} + s^{-3\nu})}{(1 + s^{-2\nu})^3} ds \]

\[ \leq (\rho n^{-\nu})^{1+1/\nu} \left( \int_0^1 s^{1+\nu} ds + \int_0^{n\rho^{-1/\nu}} s^{1-3\nu} ds \right), \]

and applying Lemma 14 with \( x = n\rho^{-1/\nu} \) gives

\[ \int_0^{n\rho^{-1/\nu}} s^{1-3\nu} ds \leq 3(n\rho^{-1/\nu})^{1-\nu} \]

so \( J_3 \leq C n^{-\nu-1} \rho^{1+1/\nu}(1 + n^{-\nu-1} \rho^{1-1/\nu}) \leq C(n^{-\nu-1} \rho^{1+1/\nu} + n^{-2\nu} \rho^2) \leq C n^{-1} \rho^2. \)

Inserting the foregoing estimates for \( J_1 \), \( J_2 \) and \( J_3 \) into (43) gives the desired estimate

\[ |I_1| \leq C n^{-1} \rho^2, \]

which completes the proof.

5. Numerical example

We consider a 1D example in which \( u = u(x,t) \) satisfies (1) with \( Au = -(\kappa u_x)_x \) for \( x \in \Omega = (-1, 1) \), subject to homogeneous Dirichlet boundary conditions \( u(\pm 1, t) = 0 \) for \( 0 < t \leq 1 \). We choose \( \kappa = 4/\pi^2 \) so the orthonormal eigenfunctions and corresponding eigenvalues of \( A \) are

\[ \phi_m(x) = \sin\left(\frac{m\pi}{2}(x+1)\right) \quad \text{and} \quad \lambda_m = m^2 \quad \text{for} \ m = 1, 2, 3, \ldots. \]

For our initial data we choose simply the constant function \( u_0(x) = \pi/4 \), which has the Fourier sine coefficients

\[ u_{0m} = \langle u_0, \phi_m \rangle = \begin{cases} m^{-1}, & m = 1, 3, 5, \ldots, \\ 0, & m = 2, 4, 6, \ldots. \end{cases} \]

Although infinitely differentiable, the function \( u_0 \) is “non-smooth” because it fails to satisfy the boundary conditions, and as a result the solution \( u(x,t) \) is discontinuous at \( x = \pm 1 \) when \( t = 0 \). In fact, if \( r < 1/4 \) then

\[ \|A^r u_0\|^2 = \sum_{m=1}^\infty (\lambda_m^r u_{0m})^2 = \sum_{j=1}^\infty (2j - 1)^{4r-1} \leq \frac{C}{1 - 4r}, \]

but if \( r \geq 1/4 \) then \( u_0 \notin D(A^r) \).

Using a closed form expression for \( \hat{u}(x,z) \), we construct a reference solution by applying a spectrally accurate numerical method [12] for inversion of the Laplace transform. To compute the discrete-time solution \( U^n \) we discretize also in space using piecewise linear finite elements on a fixed nonuniform mesh with \( M \) subintervals. In view of the discontinuity in the solution when \( t = 0 \), we concentrate the spatial grid points near \( x = \pm 1 \), but always use a constant timestep \( \Delta t = 1/N \).
Figure 3 shows the reference solution and the error in the case \( \nu = 0.75 \) using \( N = 20 \) time steps and \( M = 80 \) spatial subintervals. As expected, the error is largest at the first time level \( t_1 \) and then decays as \( t \) increases. We put \( r = \frac{1}{4} - \epsilon \) where \( \epsilon^{-1} = \max(4, \log t_n^{-1}) \), so that \( t_n^{\epsilon} \leq C \) and, by Theorem 7,

\[
\|U^n - u(t_n)\| \leq Ct_n^{\nu/4 - 1} \Delta t \sqrt{\max(1, \log t_n^{-1})} \text{ for } 0 < t_n \leq 1.
\]

Thus, ignoring the logarithm and putting \( \nu = 3/4 \), we expect to observe errors of order \( t_n^{-13/16} \Delta t \).

Figure 4 shows how the error varies with \( t_n \) for a sequence of solutions obtained by successively doubling \( N \) (and hence halving \( \Delta t \)), using a log scale. (The same spatial mesh with \( M = 1000 \) subintervals was used in all cases.) Table 1 provides an alternative view of this data, listing the weighted error and its associated convergence rate,

\[
E_N = \max_{1 \leq t_n \leq 1/2} t_n^\alpha \|U^n - u(t_n)\| \quad \text{and} \quad \rho_N = \log_2(E_N/E_{N/2}), \tag{44}
\]

so that if \( E_N \) decays like \( N^{-\rho} = \Delta t^\rho \) then \( \rho \approx \rho_N \). As expected, \( \rho_N \approx 1 \) when \( \alpha = 13/16 = 0.8125 \), but the rate deteriorates for smaller values of \( \alpha \).
Figure 4: The error $\|U^n - u(t_n)\|$ as a function of $t_n$.

Figure 5: The functions $\Phi_1$ and $\Phi_2$ from [45].
Our analysis in Section 4 does not reveal how the constant in Theorem 4 depends on the fractional diffusion exponent $\nu$, because the proof of Lemma 9 is not constructive. The factor $(1 - \nu)^{-2}$ in the estimate of Lemma 8 raises the question of whether the DG error becomes large if $\nu$ is very close to 1. We therefore investigated numerically the values of

$$
\Phi_1(\nu) = \sup_{0 < \mu < \infty} \max_{n^\nu \leq \mu - 1} n^{1-2\nu} \mu^{-2} \delta^n(\mu), \\
\Phi_2(\nu) = \sup_{0 < \mu < \infty} \sup_{n^\nu \geq \mu - 1} n^{1+\nu} \mu \delta^n(\mu),
$$

(45)
since $C = \max(\Phi_1(\nu), \Phi_2(\nu))$ is the best possible constant in Theorem 4. Figure 5 shows approximations of the graphs of $\Phi_1$ and $\Phi_2$, obtained by restricting $\mu$ to the discrete values $2^j$ for $-18 \leq j \leq 20$, and restricting $n$ to the range $1 \leq n \leq 200$. We solved (12) and (16) with $u_{0m} = 1 = U_0^m$ and $\lambda_m = \mu/\Delta t^\nu$ to compute $\delta^n(\mu) = U_m^n - u_m(t_n)$. The evaluation of $\Phi_1(\nu)$ is problematic for $\nu$ near zero because our values for $u_m(t_n)$ are not sufficiently accurate, but it seems reasonable to conjecture that $C \leq 1$ for all $\nu$.

Acknowledgement. We thank Peter Brown for help with the proof of Lemma 15.

References

[1] C-M. Chen, F. Liu, V. Anh, and I. Turner. Numerical methods for solving a two-dimensional variable-order anomalous sub-diffusion equation. Math. Comp., 81:345–366, 2012.

[2] E. Cuesta, C. Lubich, and C. Palencia. Convolution quadrature time discretization of fractional diffusive-wave equations. Math. Comp., 75:673–696, 2006.

[3] M. Cui. Compact finite difference method for the fractional diffusion equation. J. Comput. Phys., 228:7792–7804, 2009.

[4] Philippe Flajolet. Singularity analysis and asymptotics of Bernoulli sums. Theoret. Comput. Sci., 215:371–381, 1999.

[5] Walter B. Ford. Studies on divergent series and summability, and the asymptotic developments of functions defined by Maclaurin series. Chelsea Publishing Company, New York, 1960.

[6] Bangti Jin, Raytcho Lazarov, and Zhi Zhou. Error estimates for a semidiscrete finite element method for fractional order parabolic equations. SIAM J. Numer. Anal., 51:445–466, 2013.

[7] J. Klafter and I. M. Sokolov. First steps in random walks: from tools to applications. Oxford University Press, 2011.
[8] T. A. M. Langlands and B. I. Henry. The accuracy and stability of an implicit solution method for the fractional diffusion equation. *J. Comput. Phys.*, 205:719–936, 2005.

[9] Leonard Lewin. *Polylogarithms and associated functions*. North Holland, New York-Oxford, 1981.

[10] William McLean. Regularity of solutions to a time-fractional diffusion equation. *ANZIAM Journal*, 52(0), 2011.

[11] William McLean and Kassem Mustapha. Convergence analysis of a discontinuous Galerkin method for a fractional diffusion equation. *Numer. Algor.*, 52:69–88, 2009.

[12] William McLean and Vidar Thomée. Numerical solution via Laplace transforms of a fractional order evolution equation. *J. Integral Equations Appl.*, 22:57–94, 2010.

[13] William McLean, Vidar Thomée, and Lars Wahlbin. Discretization with variable time steps of an evolution equation with a positive-type memory term. *J. Comput. Appl. Math.*, 69:49–69, 1996.

[14] Kassem Mustapha. An implicit finite difference time-stepping method for a sub-diffusion equation, with spatial discretization by finite elements. *IMA J. Numer. Anal.*, 31:719–739, 2011.

[15] Kassem Mustapha and William McLean. Uniform convergence for a discontinuous Galerkin, time stepping method applied to a fractional diffusion equation. *IMA J. Numer. Anal.*, 32:906–925, 2012.

[16] Kassem Mustapha and William McLean. Superconvergence of a discontinuous Galerkin method for fractional diffusion and wave equations. *SIAM J. Numer. Anal.*, 51:491–515, 2013.

[17] J. Quintana-Murillo and S. B. Yuste. A finite difference method with non-uniform timesteps for fractional diffusion and diffusion-wave equations. *Eur. Phys. J. Special Topics*, 222:1987–1998, 2013.

[18] Vidar Thomée. *Galerkin finite element methods for parabolic problems*. Springer, 1997.

[19] David Wood. The computation of polylogarithms. Technical Report 15-92*, University of Kent, Computing Laboratory, University of Kent, Canterbury, UK, June 1992.

[20] Ya-nan Zhang, Zhi-zhong Sun, and Hong-lin Liao. Finite difference methods for the time fractional diffusion equation on non-uniform meshes. *J. Comput. Phys.*, 265:195–210, 2014.

[21] Antoni Zygmund. *Trigonometric series, Volume I*. Cambridge University Press, 1959.