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

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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 nth 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.

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1. Introduction

Consider an initial-value problem for an abstract, time-fractional diffusion equation [\[7,](#page-20-0) p. 84]

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

$$
\partial_t^{1-\nu} u(t) = \frac{\partial}{\partial t} \int_0^t \frac{(t-s)^{\nu-1}}{\Gamma(\nu)} u(s) ds
$$

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the Riemann–Liouville fractional derviative of order $1-\nu$. The linear operator A is assumed to be self-adjoint, positive-semidefinite and densely defined in H , with a complete orthonormal eigensystem ϕ_1 , ϕ_2 , ϕ_3 , We further assume that the eigenvalues of A tend to infinity. Thus,

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

where $\langle u, v \rangle$ is the inner product in H; the corresponding norm in 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 Ω , with u subject to homogeneous Dirichlet or Neumann boundary conditions on $\partial\Omega$. Our problem [\(1\)](#page-0-0) then reduces to the classical heat equation when $\nu \rightarrow 1$.

Many authors have studied techniques for the time discretization of [\(1\)](#page-0-0), but obtaining sharp error bounds has proved challenging. In studies of explicit and implicit finite difference schemes [\[1,](#page-20-1) [3,](#page-20-2) [8,](#page-21-0) [14,](#page-21-1) [17,](#page-21-2) [20\]](#page-21-3) 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,](#page-21-4) [15,](#page-21-5) 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 piecewiseconstant 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 Δt . Our previous analysis [\[11,](#page-21-4) Theorem 5] of the scheme [\(5\)](#page-2-0), in conjunction with relevant estimates [\[10\]](#page-21-7) of the derivatives of u, shows, in the special case of uniform time steps, only the sub-optimal error bound

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

In our main result, we substantially improve on [\(2\)](#page-1-0) by showing that

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

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 Δt , uniformly in t_n . For $0 < \nu \leq 1/2$, no matter how smooth u_0 a factor t_n^{2r-1} is present. To the best of our knowledge, only Cuesta et al. [\[2\]](#page-20-3) and McLean and Thomée [\[12,](#page-21-8) Theorem 3.1] have hitherto investigated the time discretization of [\(1\)](#page-0-0) 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 [\(1\)](#page-0-0). By contrast, Jin, Lazarov and Zhou [\[6\]](#page-20-4) applied a piecewise linear finite element method using a quasi-uniform partition of Ω into elements with maximum diameter h , but with no time discretization. They worked with an equivalent formulation of the fractional diffusion problem,

$$
\partial_{t,C}^{\nu} u - \nabla^2 u = 0 \quad \text{for } x \in \Omega \text{ and } 0 < t \le T,\tag{4}
$$

where $\partial_{t,C}$ denotes the Caputo fractional derivative, and proved [\[6,](#page-20-4) Theorems 3.5 and 3.7 that, for an appropriate choice of $u_h(0)$,

$$
||u_h(t) - u(t)|| + h||\nabla(u_h - u)|| \le Ct^{\nu(r-1)} \times \begin{cases} h^2 \ell_h ||A^r u_0||, & r \in \{0, 1/2\}, \\ h^2 ||A^r u_0||, & r = 1, \end{cases}
$$

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 [\[11,](#page-21-4) [13\]](#page-21-9),

$$
U^{n} - U^{n-1} + \int_{t_{n-1}}^{t_n} \partial_{t}^{1-\nu} AU(t) dt = 0 \quad \text{for } n \ge 1 \text{, with } U^{0} = u_{0}, \qquad (5)
$$

where $U^n = U(t_n^-) = \lim_{t \to t_n^-} U(t)$ 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

$$
\int_{t_{n-1}}^{t_n} \partial_t^{1-\nu} AU(t) dt = \Delta t^{\nu} \sum_{j=1}^n \beta_{n-j} AU^j,
$$

with

$$
\beta_0 = \Delta t^{-\nu} \int_{t_{n-1}}^{t_n} \frac{(t_n - t)^{\nu - 1}}{\Gamma(\nu)} dt = \frac{1}{\Gamma(1 + \nu)}
$$

and, for $j \geq 1$,

$$
\beta_j = \Delta t^{-\nu} \int_{t_{n-j-1}}^{t_{n-j}} \frac{(t_n - t)^{\nu-1} - (t_{n-1} - t)^{\nu-1}}{\Gamma(\nu)} dt = \frac{(j+1)^{\nu} - 2j^{\nu} + (j-1)^{\nu}}{\Gamma(1+\nu)}.
$$

Thus, by solving the recurrence relation

$$
(I + \beta_0 \Delta t^{\nu} A) U^n = U^{n-1} - \Delta t^{\nu} \sum_{j=1}^{n-1} \beta_{n-j} A U^j
$$
 (6)

for $n = 1, 2, 3, ...$ we may compute $U^1, U^2, U^3, ...$

In the classical limit as $\nu \rightarrow 1$, the fractional-order equation [\(1\)](#page-0-0) reduces to an abstract heat equation,

 $\partial_t u + Au = 0 \text{ for } t > 0, \text{ with } u(0) = u_0,$ (7)

and the time-stepping DG method [\(5\)](#page-2-0) reduces to the implicit Euler scheme

$$
\frac{U^n - U^{n-1}}{\Delta t} + AU^n = 0,\t\t(8)
$$

for which the following error bound holds [\[18,](#page-21-10) Theorems 7.1 and 7.2]:

$$
||U^{n} - u(t_{n})|| \leq Ct_{n}^{r-1} \Delta t ||A^{r} u_{0}|| \quad \text{for } n = 1, 2, 3, ... \text{ and } 0 \leq r \leq 1.
$$
 (9)

This result is just the limiting case as $\nu \to 1$ of our error estimate [\(3\)](#page-1-1) 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

$$
||A^r v||^2 = \sum_{m=1}^{\infty} \lambda_m^{2r} v_m^2 < \infty,
$$
\n(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 Thomée [\[18,](#page-21-10) Lemma 3.1] or [\[10,](#page-21-7) Section 3]. 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

$$
u(t) = \sum_{m=1}^{\infty} u_m(t)\phi_m, \qquad u_m(t) = \langle u(t), \phi_m \rangle,
$$
 (11)

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

$$
u'_{m} + \lambda_{m} \partial_{t}^{1-\nu} u_{m} = 0, \quad \text{for } t > 0, \text{ with } u_{m}(0) = u_{0m}, \tag{12}
$$

so that, as is well known [\[10\]](#page-21-7), $u_m(t) = E_{\nu}(-\lambda_m t^{\nu})u_{0m}$ where E_{ν} 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](#page-4-0) uses Laplace transform techniques to derive integral representations for the Fourier coefficients $U_m^n = \langle U^n, \phi_m \rangle$ and $u_m(t_n) = \langle u(t_n), \phi_m \rangle$. We show that $U_m^n - u_m(t_n) = \delta^n(\mu)u_{0m}$, where $\delta^n(\mu)$ is given by an explicit but complicated integral; thus, the error has a Fourier expansion of the form

$$
U^{n} - u(t_{n}) = \sum_{m=1}^{\infty} \delta^{n} (\lambda_{m} \Delta t^{\nu}) u_{0m} \phi_{m}, \quad u_{0m} = \langle u_{0}, \phi_{m} \rangle.
$$
 (13)

Theorem [4](#page-8-0) states a key estimate for $\delta^{n}(\mu)$, but to avoid a lengthy digression the proof is relegated to Section [4.](#page-10-0)

The main result [\(3\)](#page-1-1) of the paper is established in Section [3,](#page-9-0) where we first prove in Theorem [5](#page-9-1) that if $u_0 \in \mathcal{H}$ then the error is of order $t_n^{-1} \Delta t$, coinciding with the error estimate [\(9\)](#page-3-0) for the classical heat equation when $r = 0$. Next we prove the special case $r = \min(2, 1/\nu)$ of [\(3\)](#page-1-1) and then, in Theorem [7,](#page-10-1) deduce the general case by interpolation. The paper concludes with Section [5,](#page-17-0) 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 ν .

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 [\[11,](#page-21-4) [13\]](#page-21-9) shows that $||u(t)|| \le ||u_0||$ so $\hat{u}(z)$ exists and is analytic in the right half-plane $\Re z > 0$, and since $\mathcal{L}\{\partial_t^{1-\nu}u\} = z^{1-\nu}\hat{u}(z)$ and $\mathcal{L}{\lbrace \partial_t u \rbrace} = z\hat{u} - u_0$, it follows from [\(12\)](#page-3-1) that $z\hat{u}_m + \lambda_m z^{1-\nu}\hat{u}_m = u_{0m}$, so

$$
\hat{u}_m(z) = \frac{u_{0m}}{z + \lambda_m z^{1-\nu}}.
$$

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

$$
u_m(t_n) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} e^{zt_n} \hat{u}_m(z) \, dz = \frac{u_{0m}}{2\pi i} \int_{a-i\infty}^{a+i\infty} \frac{e^{zt_n}}{1 + \lambda_m z^{-\nu}} \, \frac{dz}{z},
$$

which, following a substitution, we may write as

$$
u_m(t_n) = \frac{u_{0m}}{2\pi i} \int_{a-i\infty}^{a+i\infty} \frac{e^{nz}}{1 + \mu z^{-\nu}} \frac{dz}{z}, \quad \text{where } \mu = \lambda_m \Delta t^{\nu}.
$$
 (14)

It follows using Jordan's lemma that

$$
u_m(t_n) = \frac{u_{0m}}{2\pi i} \int_{-\infty}^{0^+} \frac{e^{nz}}{1 + \mu z^{-\nu}} \frac{dz}{z} \quad \text{for } n \ge 1,
$$
 (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 [\(6\)](#page-2-1) used to compute the numerical solution. The Fourier coefficients $U_m^n = \langle U^n, \phi_m \rangle$ satisfy

$$
(1 + \beta_0 \Delta t^{\nu} \lambda_m) U_m^n = U_m^{n-1} - \lambda_m \Delta t^{\nu} \sum_{j=1}^{n-1} \beta_{n-j} U_m^j,
$$
 (16)

and to obtain an integral representation of U_m^n analogous to (15) we introduce the discrete-time Laplace transform

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

Again, a standard energy argument shows that $||U^n|| \le ||u_0||$ so this series converges in the right half-plane $\Re z > 0$. Multiplying [\(16\)](#page-4-2) by e^{-nz} , summing over n and using the fact that the sum in [\(16\)](#page-4-2) 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 $\psi(z) = \tilde{\beta}(z)/(1 - e^{-z}),$

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

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

where the polylogarithm [\[9,](#page-21-11) [19\]](#page-21-12) is defined by $\text{Li}_p(z) = \sum_{n=1}^{\infty} z^n/n^p$ for $|z| < 1$ and $p \in \mathbb{C}$; thus,

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

From the identity

$$
\frac{1}{n^p} = \frac{\Gamma(1-p)}{2\pi i} \int_{-\infty}^{0^+} e^{nw} w^{p-1} dw,
$$

we find, after interchanging the sum and integral, that

$$
\text{Li}_p(e^{-z}) = \frac{\Gamma(1-p)}{2\pi i} \int_{-\infty}^{0^+} \frac{w^{p-1} dw}{e^{z-w} - 1}
$$
 (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

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

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

$$
\psi(z) = \frac{\sin \pi \nu}{\pi} \int_0^\infty \frac{s^{-\nu}}{1 - e^{-z - s}} \frac{1 - e^{-s}}{s} ds \tag{23}
$$

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

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

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

Since

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

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,

$$
\mathcal{C}_{\pm} = \{ se^{\pm i\pi} : \text{for } 0 < s < \infty \},\tag{24}
$$

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 $\mathcal{C}^+ - \mathcal{C}^-$ to obtain [\(23\)](#page-5-2).

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

$$
\psi(x+iy) = \frac{1}{\Gamma(1+\nu)} \left(1 + \sum_{n=1}^{\infty} \alpha_n \cos ny - i \sum_{n=1}^{\infty} \alpha_n \sin ny \right). \tag{25}
$$

The sequence α_n is convex and tends to zero, so [\[21,](#page-21-13) pp. 183 and 228]

$$
\Re\psi(x+iy)\geq \frac{1}{2\Gamma(1+\nu)}\quad\text{and}\quad \Im\psi(x+iy)<0\quad\text{for }x\geq 0\text{ and }0
$$

and using [\(22\)](#page-5-3) we find that $\Im \psi(x \pm i\pi) = 0$ for $-\infty < x < \infty$. The polylogarithm satisfies [\[19,](#page-21-12) Equation (3.1)]

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

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

$$
\Im \psi (se^{\pm i\pi}) = \mp (1 - e^{-s}) s^{-\nu - 1} \sin \pi \nu,
$$
\n(26)

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 $x \ge 0$, and by [\(23\)](#page-5-2),

$$
\psi(x \pm i\pi) = \frac{\sin \pi \nu}{\pi} \int_0^\infty \frac{s^{-\nu}}{1 + e^{-x-s}} \frac{1 - e^{-s}}{s} ds > 0
$$

for all real x , which completes the proof.

 \Box

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 [\(17\)](#page-5-4) of \widetilde{U}_m , after interchanging the sum and integral, that for any $a > 0$,

$$
U_m^n = \frac{1}{2\pi i} \int_{a-i\pi}^{a+i\pi} e^{nz} \widetilde{U}_m(z) dz.
$$
 (27)

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 [\(18\)](#page-5-5) for $\tilde{U}_m(z)$ implies that

$$
U_m^n = \frac{u_{0m}}{2\pi i} \int_{a-i\pi}^{a+i\pi} \frac{e^{nz}}{1 + \mu\psi(z)} \frac{dz}{e^z - 1} \quad \text{for } n \ge 1.
$$
 (28)

The next lemma describes the asymptotic behaviour of ψ , and shows in par-ticular that the integrands of [\(14\)](#page-4-3) and [\(28\)](#page-7-0) are close for z near 0. In [\(29\)](#page-7-1), ζ denotes the Riemann zeta function.

Lemma 2. The function (20) satisfies

$$
\psi(z) = z^{-\nu} + \frac{1}{2}z^{1-\nu} + \frac{\zeta(-\nu)}{\Gamma(1+\nu)}z + O(z^{2-\nu}) \quad \text{as } z \to 0,
$$
 (29)

and

$$
\psi(z) = \frac{\sin \pi \nu}{\pi \nu} \left(i\pi - z \right)^{-\nu} + O(z^{-\nu - 1}) \quad \text{as } \Re(z) \to -\infty, \text{ with } 0 < \Im z < \pi. \tag{30}
$$

Proof. Flajolet [\[4,](#page-20-5) Theorem 1] shows that

$$
\text{Li}_p(e^{-z}) \sim \Gamma(1-p)z^{p-1} + \sum_{k=0}^{\infty} (-1)^k \zeta(p-k) \frac{z^k}{k!} \quad \text{as } z \to 0,
$$
 (31)

and [\(29\)](#page-7-1) follows because $e^z - 1 = z + \frac{1}{2}z^2 + O(z^3)$ as $z \to 0$. The results of Ford [\[5,](#page-20-6) Equation (17), p. 226] imply that

$$
\text{Li}_p(e^{-z}) = -\frac{(i\pi - z)^p}{\Gamma(1 + p)} + O(z^{p-1}) \quad \text{as } \Re z \to -\infty,
$$
 (32)

(see also Wood [\[19,](#page-21-12) Equation (11.2)]) which, in combination with the identity $\Gamma(1+\nu)\Gamma(1-\nu) = \pi \nu / \sin \pi \nu$, implies [\(30\)](#page-7-2). \Box

The formula for U_m^n in the next theorem matches [\(15\)](#page-4-1) for $u_m(t_n)$.

Figure 1: The integration contour $\mathcal{C}(a, M)$.

Theorem 3. The solution of [\(16\)](#page-4-2) admits the integral representation

$$
U_m^n = \frac{u_{0m}}{2\pi i} \int_{-\infty}^{0^+} \frac{e^{nz}}{1 + \mu\psi(z)} \frac{dz}{e^z - 1} \quad \text{for } n \ge 1,
$$
 (33)

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

Proof. By Lemma [1,](#page-5-6) the integrand from (28) is analytic for z inside the contour $C(a, M)$ shown in Figure [1.](#page-8-1) The contributions along $\Im z = \pm \pi$ cancel in view of the second part of [\(22\)](#page-5-3). Using [\(30\)](#page-7-2), if $\Re z \to -\infty$ then

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

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

Together, [\(15\)](#page-4-1) and [\(33\)](#page-8-2) imply that the error formula [\(13\)](#page-3-2) holds, with

$$
\delta^{n}(\mu) = \frac{1}{2\pi i} \int_{-\infty}^{0^{+}} e^{nz} \left(\frac{1}{1 + \mu \psi(z)} \frac{z}{e^{z} - 1} - \frac{1}{1 + \mu z^{-\nu}} \right) \frac{dz}{z}
$$
(34)

for $0 < \mu < \infty$, and with $\delta^n(0) = 0$ because if $\lambda_m = 0$ then $u_m(t_n) = u_{0m} = U_m^n$ for all *n*. The following estimate for $\delta^n(\mu)$ is the key to proving our error estimates, but the lengthy proof is deferred until Section [4.](#page-10-0)

Theorem 4. Let $0 < \nu < 1$. The sequence [\(34\)](#page-8-3) satisfies

$$
|\delta^{n}(\mu)| \leq Cn^{-1} \min((\mu n^{\nu})^{2}, (\mu n^{\nu})^{-1}) \quad \text{for } n = 1, 2, 3, \dots \text{ and } 0 < \mu < \infty.
$$

Proof. Follows from Theorems [12](#page-12-0) and [16.](#page-14-0)

 \Box

We remark that in the limiting case $\nu \rightarrow 1$, when our method reduces to the classical implicit Euler scheme [\(8\)](#page-2-2) for the heat equation [\(7\)](#page-2-3), it is readily seen that the error representation [\(13\)](#page-3-2) holds with $\delta^{n}(\mu) = (1 + \mu)^{-n} - e^{-n\mu}$, and that $0 \leq \delta^n(\mu) \leq Cn^{-1} \min((\mu n)^2, (\mu n)^{-1}),$ consistent with Theorem [4.](#page-8-0)

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 $u_0 \in \mathcal{H}$, the solutions of [\(1\)](#page-0-0) and [\(5\)](#page-2-0) satisfy

$$
||U^{n} - u(t_{n})|| \leq Ct_{n}^{-1} \Delta t ||u_{0}|| \quad \text{for } n = 1, 2, 3, \dots
$$

Proof. Theorem [4](#page-8-0) implies that $|\delta^n(\mu)| \leq Cn^{-1}$ uniformly for $0 < \mu < \infty$, and since the ϕ_m are orthonormal, we see from [\(13\)](#page-3-2) that

$$
||U^{n} - u(t_{n})||^{2} = \sum_{m=1}^{\infty} \left[\delta^{n} (\lambda_{m} \Delta t^{\nu}) u_{0m} \right]^{2} \le (Cn^{-1})^{2} \sum_{m=1}^{\infty} u_{0m}^{2} = (Cn^{-1} || u_{0} ||)^{2}.
$$
\n(35)

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

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

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

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

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

$$
\begin{aligned} |\delta^n(\lambda_m \Delta t^\nu)| &\leq C t_n^{-1} \Delta t \, \min\left((\lambda_m t_n^\nu)^2, (\lambda_m t_n^\nu)^{-1} \right) \\ &= C t_n^{2\nu - 1} \Delta t \, \lambda_m^2 \min\left(1, (\lambda_m t_n^\nu)^{-3} \right) \leq C t_n^{2\nu - 1} \Delta t \, \lambda_m^2, \end{aligned}
$$

so by [\(10\)](#page-3-3) and [\(35\)](#page-9-2),

$$
||U^{n} - u(t_{n})||^{2} \leq \sum_{m=1}^{\infty} (C t_{n}^{2\nu - 1} \Delta t \lambda_{m}^{2} u_{0m})^{2} = (C t_{n}^{2\nu - 1} \Delta t ||A^{2} u_{0}||)^{2},
$$

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 $n^{-1} = \Delta t \lambda_m^{1/\nu} (\lambda_m t_n^{\nu})^{-1/\nu}$ implies that

$$
|\delta^n(\lambda_m \Delta t^{\nu})| \le C \Delta t \lambda_m^{1/\nu} \min\left((\lambda_m t_n^{\nu})^{2-1/\nu}, (\lambda_m t_n^{\nu})^{-1-1/\nu}\right) \le C \Delta t \lambda_m^{1/\nu}.
$$

 \Box

We are now ready to prove our main result.

Theorem 7. The solutions of (1) and (5) satisfy

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

Proof. If $0 < \nu \leq 1/2$ and $0 < \theta < 1$, then by interpolation

$$
||U^{n} - u(t_{n})|| \leq C \big(t_{n}^{-1} \Delta t\big)^{1-\theta} \big(t_{n}^{2\nu-1} \Delta t\big)^{\theta} ||A^{2\theta} u_{0}|| = C t_{n}^{2\nu\theta-1} \Delta t ||A^{2\theta} u_{0}||,
$$

and the estimate follows by putting $r = 2\theta$. Similarly, if $1/2 \leq \nu < 1$, then

$$
||U^{n} - u(t_{n})|| \leq C (t_{n}^{-1} \Delta t)^{1-\theta} \Delta t^{\theta} ||A^{\theta/\nu} u_{0}|| = C t_{n}^{\theta-1} \Delta t ||A^{\theta/\nu} u_{0}||,
$$

and the estimate follows by putting $r = \theta/\nu$.

\Box

4. Technical proofs

It remains to prove Theorem [4.](#page-8-0) 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_{ν} may depend on the fractional diffusion exponent ν .

Since the integrand of [\(34\)](#page-8-3) is $O(z^{\nu-1})$ as $z \to 0$, we may collapse the Hankel contour onto $\mathcal{C}_+ - \mathcal{C}_-$, for \mathcal{C}_\pm given by [\(24\)](#page-6-0). In this way, defining

$$
\psi_{\pm}(s) = \psi(se^{\pm i\pi}) \quad \text{for } 0 < s < \infty,
$$

we find that

$$
\int_{\mathcal{C}_{\pm}} e^{nz} \left(\frac{1}{1 + \mu \psi(z)} \frac{z}{e^z - 1} - \frac{1}{1 + \mu z^{-\nu}} \right) \frac{dz}{z}
$$
\n
$$
= \int_0^\infty e^{-ns} \left(\frac{1}{1 + \mu \psi_{\pm}(s)} \frac{s}{1 - e^{-s}} - \frac{1}{1 + \mu s^{-\nu} e^{\mp i \pi \nu}} \right) \frac{ds}{s}.
$$

By [\(22\)](#page-5-3) and [\(26\)](#page-6-1),

$$
\psi_{-}(s) = \overline{\psi_{+}(s)}
$$
 and $\Im \psi_{\pm}(s) = \mp (1 - e^{-s}) s^{-\nu - 1} \sin \pi \nu,$ (36)

so

$$
\frac{1}{1+\mu \psi_+(s)}-\frac{1}{1+\mu \psi_-(s)}=\frac{2i\mu \Im \psi_-(s)}{|1+\mu \psi_\pm(s)|^2}=\frac{2i\mu s^{-\nu}\sin \pi \nu}{|1+\mu \psi_\pm(s)|^2}\,\frac{1-e^{-s}}{s},
$$

and similarly,

$$
\frac{1}{1+\mu s^{-\nu}e^{-i\pi\nu}}-\frac{1}{1+\mu s^{-\nu}e^{i\pi\nu}}=\frac{2i\mu s^{-\nu}\sin\pi\nu}{|1+\mu s^{-\nu}e^{\mp i\pi\nu}|^2}.
$$

Thus, the representation [\(34\)](#page-8-3) implies

$$
\delta^{n}(\mu) = \frac{\sin \pi \nu}{\pi} \int_0^{\infty} e^{-ns} \mu s^{-\nu} \left(\frac{1}{|1 + \mu \psi_+(s)|^2} - \frac{1}{|1 + \mu s^{-\nu} e^{-i\pi \nu}|^2} \right) \frac{ds}{s} . \quad (37)
$$

We will estimate this integral with the help of the following sequence of lemmas.

Lemma 8. If $X \ge 0$ then $|1 + Xe^{\pm i\pi\nu}|^{-2} \le (1 - \nu)^{-2}(1 + X^2)^{-1}$.

Proof. Since $0 \le 2X/(1 + X^2) \le 1$,

$$
\frac{|1+Xe^{\pm i\pi\nu}|^2}{1+X^2} = \frac{|e^{\mp i\pi\nu} + X|^2}{1+X^2} = 1 + \frac{2X}{1+X^2} \cos \pi\nu \ge \min(1, 1 + \cos \pi\nu),
$$

and the result follows because $1 + \cos \pi \nu = 2 \cos^2(\pi \nu/2) \geq 2(1 - \nu)^2$. \Box **Lemma 9.** If $\mu \ge 0$ and $s > 0$, then $|1 + \mu \psi_{\pm}(s)|^{-2} \le C_{\nu} (1 + \mu^2 s^{-2\nu})^{-1}$.

Proof. Lemma [2](#page-7-3) implies that

$$
\psi_{\pm}(s) = e^{\mp i\pi\nu}(s^{-\nu} - \frac{1}{2}s^{1-\nu}) - \frac{\zeta(-\nu)}{\Gamma(1+\nu)}s + O(s^{2-\nu}) \quad \text{as } s \to 0 \tag{38}
$$

and

$$
\psi_{\pm}(s) = \frac{\sin \pi \nu}{\pi \nu} s^{-\nu} + O(s^{-\nu - 1}) \text{ as } s \to \infty.
$$
\n(39)

Thus, if we define $\phi(s) = s^{\nu} \psi_+(s)$ for $0 < s < \infty$, with

$$
\phi(0) = e^{-i\pi\nu} \quad \text{and} \quad \phi(\infty) = \frac{\sin \pi\nu}{\pi\nu},\tag{40}
$$

then ϕ is continuous on the one-point compactification $[0, \infty]$ of the closed halfline [0, ∞). Put $X = \mu s^{-\nu}$ and define

$$
f(s, X) = \frac{|1 + \mu\psi_+(s)|^2}{1 + X^2} = \frac{|1 + X\phi(s)|^2}{1 + X^2}
$$

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) ,

$$
\Im \phi(s) = -\frac{1 - e^{-s}}{s} \sin \pi \nu < 0 \quad \text{for } 0 < s < \infty,\tag{41}
$$

and $\Im \phi(0) = -\sin \pi \nu < 0$ by [\(40\)](#page-11-0), 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 $0 \le s \le \infty$. Finally, [\(40\)](#page-11-0) and [\(41\)](#page-11-1) imply that $f(s,\infty) = |\phi(s)|^2 > 0$ for $0 \le s \le \infty$. \Box

Lemma 10. For $\mu \geq 0$ and $s > 0$,

$$
|1 + \mu s^{-\nu} e^{\mp i\pi\nu}|^2 - |1 + \mu \psi_{\pm}(s)|^2
$$

= $\mu B_{+}(s)(1 + \mu s^{-\nu} e^{i\pi\nu}) + \mu B_{-}(s)(1 + \mu \psi_{+}(s)) = \mu B_{1}(s) + \mu^{2} B_{2}(s),$

where $B_{\pm}(s) = s^{-\nu}e^{\mp i\pi\nu} - \psi_{\pm}(s)$ and

$$
B_1(s) = B_+(s) + B_-(s) = 2(s^{-\nu}\cos\pi\nu - \Re\psi_\pm(s)),
$$

\n
$$
B_2(s) = B_+(s)s^{-\nu}e^{i\pi\nu} + B_-(s)\psi_+(s) = s^{-2\nu} - \psi_+(s)\psi_-(s).
$$

Proof. Put $a = \mu s^{-\nu} e^{\mp i\pi\nu}$ and $b = \mu \psi_{\pm}$ in the identities

$$
|1 + a|^2 - |1 + b|^2 = (a - b)(1 + \bar{a}) + (\bar{a} - \bar{b})(1 + b)
$$

= $(a - b) + (\bar{a} - \bar{b}) + (a\bar{a} - b\bar{b}).$

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

Lemma 11. $As s \rightarrow 0$,

$$
B_{\pm}(s) = O(s^{1-\nu}),
$$
 $B_1(s) = s^{1-\nu} \cos \pi \nu + O(s),$ $B_2(s) = s^{1-2\nu} + O(s^{1-\nu}),$

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 [\(38\)](#page-11-2) and [\(39\)](#page-11-3).

 \Box

 \Box

 \Box

We are now ready to prove the easier half of Theorem [4.](#page-8-0)

Theorem 12. For $0 < \mu < \infty$ and $n = 1, 2, 3, \ldots$, the sequence [\(34\)](#page-8-3) satisfies

$$
|\delta^n(\mu)| \le C_\nu n^{-1} \rho^{-1} \quad \text{if } \rho = \mu n^\nu.
$$

Proof. From [\(37\)](#page-10-3) and Lemma [10,](#page-11-4) we see that $\delta^{n}(\mu)$ equals

$$
\frac{\sin \pi \nu}{\pi} \int_0^\infty e^{-ns} \mu s^{-\nu} \frac{\mu B_+(s) \left(1 + \mu s^{-\nu} e^{i \pi \nu} \right) + \mu B_-(s) \left(1 + \mu \psi_+(s)\right)}{|1 + \mu s^{-\nu} e^{i \pi \nu}|^2|1 + \mu \psi_+(s)|^2} \frac{ds}{s},
$$

and thus, by Lemmas [8](#page-11-5) and [9,](#page-11-6)

$$
|\delta^n(\mu)| \leq C_\nu \int_0^\infty e^{-ns} \mu s^{-\nu} \, \frac{\mu |B_{\pm}(s)|}{(1 + \mu^2 s^{-2\nu})^{3/2}} \, \frac{ds}{s}.
$$

Lemma [11](#page-12-1) implies that $|B_{\pm}(s)| \leq C_{\nu} \min(s^{1-\nu}, s^{-\nu}) = C_{\nu} s^{-\nu} \min(s, 1),$ so

$$
|\delta^{n}(\mu)| \le C_{\nu} \int_0^{\infty} g_n(s,\mu) \, ds \quad \text{where} \quad g_n(s,\mu) = e^{-ns} \mu^2 \, \frac{s^{-2\nu - 1} \min(s,1)}{(1 + \mu^2 s^{-2\nu})^{3/2}}.
$$

The estimate for $\delta^n(\mu)$ follows because

$$
\int_0^1 g_n(s,\mu) \, ds \le \int_0^1 e^{-ns} \, \frac{s^{\nu}}{\mu} \, ds = \frac{n^{-1-\nu}}{\mu} \int_0^n e^{-s} s^{\nu} \, ds \le \frac{\Gamma(1+\nu)}{n\rho}
$$

and

$$
\int_1^\infty g_n(s,\mu)\,ds \le \int_1^\infty e^{-ns}\frac{s^{\nu-1}}{\mu}\,ds \le \int_1^\infty \frac{e^{-ns}}{\mu}\,ds = \frac{n^\nu}{\rho}\,\frac{e^{-n}}{n} \le \frac{C}{n\rho}.
$$

Figure 2: The contour $\mathcal{C}(\epsilon, R)$ used in the proof of Lemma [15.](#page-13-0)

Establishing the behaviour of $\delta^n(\mu)$ when $\rho = \mu n^{\nu}$ is small turns out to be more delicate, and relies on three additional lemmas.

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

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

$$
f'(x) > 0 \text{ for } 0 < x < x^* \quad \text{and} \quad f'(x) < 0 \text{ for } x^* < x < 1,\tag{42}
$$

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

$$
f(x) \le f(x^*) = \frac{(x^*)^{1-2\nu}}{\nu} = \frac{(x^*)^{\nu}}{1-2\nu} \le 3.
$$

If $\nu = 1/3$, then $f(x) = x^{1/3} \log x^{-1}$ and [\(42\)](#page-13-1) holds with $x^* = e^{-3}$, implying that $f(x) \le f(x^*) = 3e^{-1} \le 3$. If $1/3 < \nu < 1/2$, then [\(42\)](#page-13-1) holds with $x^* =$ $[(1-2\nu)/\nu]^{1/(3\nu-1)} < 1$ and again $f(x) \le f(x^*) = (x^*)^{1-2\nu}/\nu \le 3$. Finally, if $\nu = 0$ then $f(x) = 1 - x \le 1$, and if $\nu = 1/2$ then $f(x) = 2(1 - x^{1/2}) \le 2$.

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

Proof. Make the substitutions $x' = x^{-1}$, $s' = s^{-1}$, $\nu' = 1 - \nu$ in Lemma [13.](#page-13-2)

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

$$
I = \int_0^\infty f(x) \, dx \quad \text{and} \quad f(x) = \frac{1 - px}{(x^2 - 2px + 1)^2} \, x^{1/\nu}.
$$

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 $\alpha_{\pm} = p \pm iq = e^{i\pi(1 \mp \nu)}$ and $q = \sqrt{1-p^2} = \sin \pi \nu$. Thus, f has double poles at $z = \alpha_+$ and at α_- . Moreover, since $1 < 1/\nu < 2$ we see that $f(z) = o(|z|^{-1})$ as $|z| \to \infty$, and that $f(z) = O(|z|)$ as $|z| \to 0$. After integrating around the contour $\mathcal{C}(\epsilon, R)$ shown in Figure [2](#page-13-3) and sending $\epsilon \to 0^+$ and $R \to \infty$, we conclude that

$$
\frac{1 - e^{i2\pi/\nu}}{2\pi i} I = \underset{z = \alpha_+}{\text{res}} f(z) + \underset{z = \alpha_-}{\text{res}} f(z).
$$

Since $(z - \alpha_{\pm})^2 f(z) = (1 - pz)z^{1/\nu}/(z - \alpha_{\mp})^2$ and $\alpha_{\pm}^{1/\nu} = -e^{i\pi/\nu} = \alpha_{-}^{1/\nu}$,

$$
\mathop{\rm res}_{z=\alpha_{\pm}} f(z) = \lim_{z \to \alpha_{\pm}} \frac{d}{dz}(z - \alpha_{\pm})^2 f(z) = \frac{d}{dz} \frac{(1 - pz)z^{1/\nu}}{(z - \alpha_{\mp})^2} \bigg|_{z=\alpha_{\pm}} = \mp i \frac{1 - \nu}{\nu} \frac{e^{i\pi/\nu}}{4q},
$$

showing that the residues cancel, and therefore $I = 0$ because $e^{i2\pi/\nu} \neq 1$. \Box

Our final result for this section completes the proof of Theorem [4,](#page-8-0) and hence of the error estimates of Section [3.](#page-9-0)

Theorem 16. For $0 < \mu < \infty$ and $n = 1, 2, 3, \ldots$, the sequence [\(34\)](#page-8-3) satisfies

$$
|\delta^n(\mu)| \le C_\nu n^{-1} \rho^2 \quad \text{if } \rho = \mu n^\nu \le 1.
$$

Proof. By Lemma [11,](#page-12-1)

$$
\mu B_1(s) + \mu^2 B_2(s) = s(\mu s^{-\nu} \cos \pi \nu + (\mu s^{-\nu})^2 + O(\mu + \mu^2 s^{-\nu})) \text{ as } s \to 0^+,
$$

and
$$
\mu B_1(s) + \mu^2 B_2(s) = O(\mu s^{-\nu} + \mu^2 s^{-2\nu}) \text{ as } s \to \infty, \text{ so (37) implies that}
$$

$$
|\delta^{n}(\mu)| = \left| \frac{\sin \pi \nu}{\pi} \int_0^{\infty} e^{-ns} \mu s^{-\nu} \frac{\mu B_1(s) + \mu^2 B_2(s)}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2 |1 + \mu \psi_+(s)|^2} \frac{ds}{s} \right|
$$

$$
\leq \frac{\sin \pi \nu}{\pi} (|I_1| + C_{\nu} I_2 + C_{\nu} I_3),
$$

where, using Lemmas [8](#page-11-5) and [9,](#page-11-6)

$$
I_1 = \int_0^1 e^{-ns} \mu s^{-\nu} \frac{\mu s^{-\nu} \cos \pi \nu + (\mu s^{-\nu})^2}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2 |1 + \mu \psi_+(s)|^2} ds,
$$

\n
$$
I_2 = \int_0^1 e^{-ns} \mu s^{-\nu} \frac{\mu + \mu^2 s^{-\nu}}{(1 + \mu^2 s^{-2\nu})^2} ds, \quad I_3 = \int_1^\infty e^{-ns} \mu s^{-\nu} \frac{\mu s^{-\nu} + \mu^2 s^{-2\nu}}{(1 + \mu^2 s^{-2\nu})^2} \frac{ds}{s}.
$$

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 $f(x) \le \min(2x, x^{-2})$ we have $f(\rho s^{-\nu}) \le C \min(\rho^{-2} s^{2\nu}, \rho s^{-\nu})$ and thus

$$
n^{1+\nu} \rho^{-1} I_2 \le C \rho^{-2} \int_0^{\rho^{1/\nu}} e^{-s} s^{2\nu} ds + C \rho \int_{\rho^{1/\nu}}^n e^{-s} s^{-\nu} ds
$$

\n
$$
\le C \int_0^{\rho^{1/\nu}} e^{-s} ds + C \rho \int_{\rho^{1/\nu}}^1 s^{-\nu} ds + C \rho \int_1^\infty e^{-s} ds
$$

\n
$$
\le C \rho^{1/\nu} + C(1-\nu)^{-1} \rho + C \rho \le C(1-\nu)^{-1} \rho + C \rho^{1/\nu} \le C_{\nu} \rho,
$$

implying $I_2 \n\t\le C_\nu n^{-1-\nu} \rho^2 \le C_\nu n^{-1} \rho^2$. Noting that $\mu = \rho n^{-\nu} \le 1$, we have

$$
I_3 \le \int_1^\infty e^{-ns} \mu^2 s^{-2\nu - 1} ds \le \mu^2 \int_1^\infty e^{-ns} ds = \mu^2 \frac{e^{-n}}{n} \le n^{-1} \mu^2 = n^{-1 - 2\nu} \rho^2,
$$

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

$$
I_1 \le C_{\nu} \int_0^1 e^{-ns} g(\mu s^{-\nu}) ds = C_{\nu} n^{-1} \int_0^n e^{-s} g(\rho s^{-\nu}) ds.
$$

Since $g(x) \le \min(2x^2, x^{-2} \cos \pi \nu + x^{-1})$ we have

$$
g(\rho s^{-\nu}) \leq C \min \left(\rho^{-1} s^{\nu}, \rho^2 s^{-2\nu} \cos \pi \nu + \rho^3 s^{-3\nu} \right)
$$

and hence $\int_0^n e^{-s} g(\rho s^{-\nu}) ds$ is bounded by

$$
C\rho^{-1} \int_0^{\rho^{1/\nu}} s^{\nu} ds + C\rho^2 \cos \pi \nu \int_{\rho^{1/\nu}}^n e^{-s} s^{-2\nu} ds + C\rho^3 \int_{\rho^{1/\nu}}^n e^{-s} s^{-3\nu} ds
$$

$$
\leq C\rho^{1/\nu} + C\rho^2 \int_{\rho^{1/\nu}}^1 (1 - 2\nu) s^{-2\nu} ds + C\rho^3 \int_{\rho^{1/\nu}}^1 s^{-3\nu} ds + C\rho^2 \int_1^\infty e^{-s} ds.
$$

Applying Lemma [13](#page-13-2) with $x = \rho^{1/\nu}$ and noting that $1/\nu > 2$, it follows that $\int_0^{\hat{n}} e^{-s} g(\rho s^{-\nu}) ds \leq C(\rho^{1/\nu} + \rho^2)$ 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 $I_1 \n\t\le C_\nu n^{-1} \rho^2$. Thus, assume now that $1/2 < \nu < 1$ and note $\cos \pi \nu < 0$. Since

$$
\frac{e^{-ns}}{|1 + \mu s^{-\nu} e^{i\pi\nu}|^2 |1 + \mu \psi_+(s)|^2} = \frac{1}{|1 + \mu s^{-\nu} e^{i\pi\nu}|^4}
$$

$$
- \frac{1 - e^{-ns}}{|1 + \mu s^{-\nu} e^{i\pi\nu}|^2 |1 + \mu \psi_+(s)|^2} + \frac{|1 + \mu s^{-\nu} e^{i\pi\nu}|^2 - |1 + \mu \psi_+(s)|^2}{|1 + \mu s^{-\nu} e^{i\pi\nu}|^4 |1 + \mu \psi_+(s)|^2}
$$

and, by Lemma [15,](#page-13-0)

$$
\int_0^1 \frac{(\mu s^{-\nu})^2 \cos \pi \nu + (\mu s^{-\nu})^3}{|1 + \mu s^{-\mu} e^{i\pi \nu}|^4} ds = \mu^{1/\nu} \int_0^{\mu^{-1/\nu}} \frac{s^{-2\nu} \cos \pi \nu + s^{-3\nu}}{|1 + s^{-\nu} e^{i\pi \nu}|^4} ds
$$

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

we have

$$
|I_1| \le C_\nu (J_1 + J_2 + J_3), \tag{43}
$$

where

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

\n
$$
J_2 = \int_0^1 (1 - e^{-ns}) \frac{(\mu s^{-\nu})^2 |\cos \pi \nu| + (\mu s^{-\nu})^3}{(1 + \mu^2 s^{-2\nu})^2} ds,
$$

\n
$$
J_3 = \int_0^1 (|1 + \mu s^{-\nu} e^{i\pi \nu}|^2 - |1 + \mu \psi_+(s)|^2) \frac{(\mu s^{-\nu})^2 |\cos \pi \nu| + (\mu s^{-\nu})^3}{(1 + \mu^2 s^{-2\nu})^3} ds.
$$

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

$$
J_1 \le Cn^{-1} \rho^{1/\nu} \int_{n\rho^{-1/\nu}}^{\infty} \left((2\nu - 1)s^{-2\nu} + s^{-3\nu} \right) ds
$$

\n
$$
\le Cn^{-1} \rho^{1/\nu} \left[(n\rho^{-1/\nu})^{1-2\nu} + (n\rho^{-1/\nu})^{1-3\nu} \right]
$$

\n
$$
= Cn^{-2\nu} \rho^2 + Cn^{-3\nu} \rho^3 \le Cn^{-1} \rho^2.
$$

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

$$
\int_0^{n\rho^{-1/\nu}} (1 - e^{-\rho^{1/\nu} s}) \frac{s^{-2\nu} |\cos \pi \nu| + s^{-3\nu}}{(1 + s^{-2\nu})^2} ds \le C \int_0^1 \frac{(1 - e^{-\rho^{1/\nu} s}) s^{-3\nu}}{(1 + s^{-2\nu})^2} ds
$$

+ $C \int_1^{n\rho^{-1/\nu}} (1 - e^{-\rho^{1/\nu} s}) (s^{-2\nu} (\nu - \frac{1}{2}) + s^{-3\nu}) ds$
 $\le C \rho^{1/\nu} \int_0^1 s^{\nu+1} ds + C \int_{\rho^{1/\nu}}^n (1 - e^{-s}) (\rho^3 s^{-3\nu} + (\nu - \frac{1}{2}) \rho^2 s^{-2\nu}) ds.$

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

$$
J_2 \leq Cn^{-1} \rho^{1/\nu} \left(\rho^{1/\nu} + C\rho^{3-1/\nu} + \nu^{-1} \rho^2 \log \rho^{-1} \right) \leq C_{\nu} n^{-1} \rho^2.
$$

Third, by Lemmas [10](#page-11-4) and [11,](#page-12-1)

$$
J_3 \le \int_0^1 (\mu s^{1-\nu} + \mu^2 s^{1-2\mu}) \frac{(\mu s^{-\nu})^2 + (\mu s^{-\nu})^3}{(1+\mu s^{-\nu})^3} ds
$$

= $\mu^{1+1/\nu} \int_0^{\mu^{-1/\nu}} \frac{s(s^{-\nu} + s^{-2\nu})(s^{-2\nu} + s^{-3\nu})}{(1+s^{-2\nu})^3} ds$
 $\le (\rho n^{-\nu})^{1+1/\nu} \left(\int_0^1 s^{1+\nu} ds + \int_1^{n\rho^{-1/\nu}} s^{1-3\nu} ds \right),$

and applying Lemma [14](#page-13-4) with $x = n\rho^{-1/\nu}$ gives $\int_1^{n\rho^{-1/\nu}} s^{1-3\nu} ds \le 3(n\rho^{-1/\nu})^{1-\nu}$ so $J_3 \leq C n^{-\nu-1} \rho^{1+1/\nu} (1+n^{1-\nu} \rho^{1-1/\nu}) \leq C (n^{-\nu-1} \rho^{1+1/\nu} + n^{-2\nu} \rho^2) \leq C n^{-1} \rho^2$. Inserting the foregoing estimates for J_1 , J_2 and J_3 into [\(43\)](#page-16-0) gives the desired estimate $|I_1| \leq Cn^{-1}\rho^2$, which completes the proof. \Box

5. Numerical example

We consider a 1D example in which $u = u(x, t)$ satisfies [\(1\)](#page-0-0) 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

$$
\phi_m(x) = \sin \frac{m\pi}{2}(x+1)
$$
 and $\lambda_m = m^2$ for $m = 1, 2, 3, ...$

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

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

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

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

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 [\[12\]](#page-21-8) for inversion of the Laplace transform. To compute the discrete-time solution $Uⁿ$ 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: Reference solution (left) and error (right).

N	$\alpha = 0.6$		$\alpha = 0.7$		$\alpha = 13/16$	
80	$2.14e-03$		$1.48e-03$		$1.16e-03$	
160	$1.24e-03$	0.788	7.94e-04	0.894	$5.91e-04$	0.978
320	$7.20e-04$	0.787	$4.29e-04$	0.888	$2.98e-04$	0.988
640	$4.17e-04$ 0.787		$2.32e-04$	0.887	$1.50e-04$ 0.992	
1280	$2.42e-04$ 0.787		$1.25e-04$ 0.887		7.53e-05	0.993

Table 1: Weighted errors and observed convergence rates from [\(44\)](#page-18-0).

Figure [3](#page-18-1) 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 $t_n^{-\epsilon} \le C$ and, by Theorem [7,](#page-10-1)

$$
||U^{n} - u(t_{n})|| \leq Ct_{n}^{\nu/4 - 1} \Delta t \sqrt{\max(1, \log t_{n}^{-1})} \quad \text{for } 0 < t_{n} \leq 1.
$$

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

Figure [4](#page-19-0) shows how the error varies with t_n for a sequence of solutions obtained by successively doubling N (and hence halving Δt), using a log scale. (The same spatial mesh with $M = 1000$ subintervals was used in all cases.) Table [1](#page-18-2) provides an alternative view of this data, listing the weighted error and its associated convergence rate,

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

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 α .

Figure 4: The error $||U^n - u(t_n)||$ as a function of t_n .

Figure 5: The functions Φ_1 and Φ_2 from [\(45\)](#page-20-7).

Our analysis in Section [4](#page-10-0) does not reveal how the constant in Theorem [4](#page-8-0) depends on the fractional diffusion exponent ν , because the proof of Lemma [9](#page-11-6) is not constructive. The factor $(1 - \nu)^{-2}$ in the estimate of Lemma [8](#page-11-5) raises the question of whether the DG error becomes large if ν is very close to 1. We therefore investigated numerically the values of

$$
\Phi_1(\nu) = \sup_{0 < \mu < \infty} \max_{n^{\nu} \le \mu^{-1}} n^{1 - 2\nu} \mu^{-2} \delta^n(\mu),
$$
\n
$$
\Phi_2(\nu) = \sup_{0 < \mu < \infty} \sup_{n^{\nu} \ge \mu^{-1}} n^{1 + \nu} \mu \delta^n(\mu),
$$
\n
$$
(45)
$$

since $C = \max(\Phi_1(\nu), \Phi_2(\nu))$ is the best possible constant in Theorem [4.](#page-8-0) Fig-ure [5](#page-19-1) shows approximations of the graphs of Φ_1 and Φ_2 , obtained by restricting μ to the discrete values 2^j for $-18 \leq j \leq 20$, and resticting n to the range $1 \leq n \leq 200$. We solved [\(12\)](#page-3-1) and [\(16\)](#page-4-2) with $u_{0m} = 1 = U_m^0$ 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 ν 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 ν .

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