# 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 *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.

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#### 1. Introduction

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

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

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

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 tusing 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  $\Delta t$ . 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

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

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

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

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

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

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

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, 13],

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

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  $t_{n-1} < t \le t_n$ . Since we do not consider any spatial discretization, U is a semidiscrete solution with values in  $\mathcal{H}$ . 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  $j \ge 1$ ,

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

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  $\nu \to 1$ , the fractional-order equation (1) reduces to an abstract heat equation,

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

and the time-stepping DG method (5) reduces to the implicit Euler scheme

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

for which the following error bound holds [18, Theorems 7.1 and 7.2]:

$$||U^n - u(t_n)|| \le Ct_n^{r-1}\Delta t ||A^r u_0|| \quad \text{for } n = 1, 2, 3, \dots \text{ and } 0 \le r \le 1.$$
(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  $r \ge 0$ , 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

$$||A^{r}v||^{2} = \sum_{m=1}^{\infty} \lambda_{m}^{2r} v_{m}^{2} < \infty,$$
(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" vis. When  $\mathcal{H} = L_2(\Omega)$  the functions in  $D(A^r)$  may have to satisfy compatibility conditions on  $\partial\Omega$ ; see Thomée [18, Lemma 3.1] or [10, 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

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

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

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

so that, as is well known [10],  $u_m(t) = E_{\nu}(-\lambda_m t^{\nu})u_{0m}$  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  $U_m^n = \langle U^n, \phi_m \rangle$  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 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  $\mathcal{L}\{\partial_t^{1-\nu}u\} = z^{1-\nu}\hat{u}(z)$ and  $\mathcal{L}\{\partial_t u\} = z\hat{u} - u_0$ , it follows from (12) that  $z\hat{u}_m + \lambda_m z^{1-\nu}\hat{u}_m = u_{0m}$ , so

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

Thus, the Laplace inversion formula gives, for  $n \ge 1$  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) 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

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

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

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

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

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

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

$$\operatorname{Li}_{p}(e^{-z}) = \frac{\Gamma(1-p)}{2\pi i} \int_{-\infty}^{0^{+}} \frac{w^{p-1} \, dw}{e^{z-w} - 1}$$
(21)

for  $\Re z$  sufficiently large. Thus,  $\operatorname{Li}_p(e^{-z})$  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

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

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

so that  $\arg(w) = \pm \pi$  if  $w \in \mathcal{C}_{\pm}$ . 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).

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

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

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)]

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

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

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

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

for all real x, which completes the proof.

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  $\widetilde{U}_m$ , 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) for  $\widetilde{U}_m(z)$  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  $\psi$ , 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

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

and

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

*Proof.* Flajolet [4, Theorem 1] shows that

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

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

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

(see also Wood [19, 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  $U_m^n$  in the next theorem matches (15) for  $u_m(t_n)$ .



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

**Theorem 3.** The solution of (16) 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, the integrand from (28) is analytic for z inside the contour  $\mathcal{C}(a, M)$  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

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

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

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

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

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

*Proof.* Follows from Theorems 12 and 16.

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  $0 \le \delta^n(\mu) \le Cn^{-1} \min((\mu n)^2, (\mu n)^{-1})$ , 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  $u_0 \in \mathcal{H}$ , the solutions of (1) and (5) satisfy

$$||U^n - u(t_n)|| \le Ct_n^{-1}\Delta t ||u_0||$$
 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

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

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  $0 < \nu \le 1/2$  and  $A^2 u_0 \in \mathcal{H}$ , then  $\|U^n - u(t_n)\| \le C t_n^{2\nu - 1} \Delta t \|A^2 u_0\| \le C \Delta t^{2\nu} \|A^2 u_0\|.$ 

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  $\lambda_m \Delta t^{\nu} n^{\nu} = \lambda_m t_n^{\nu}$ ,

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

so by (10) and (35),

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

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

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

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We are now ready to prove our main result.

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

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

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

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

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

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

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

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  $\mathcal{C}_+ - \mathcal{C}_-$ , for  $\mathcal{C}_\pm$  given by (24). In this way, defining

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

we find that

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

By (22) and (26),

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

 $\mathbf{SO}$ 

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

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) implies

$$\delta^{n}(\mu) = \frac{\sin \pi\nu}{\pi} \int_{0}^{\infty} e^{-ns} \mu s^{-\nu} \left( \frac{1}{|1 + \mu\psi_{+}(s)|^{2}} - \frac{1}{|1 + \mu s^{-\nu} e^{-i\pi\nu}|^{2}} \right) \frac{ds}{s}.$$
 (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  $1 + \cos \pi \nu = 2\cos^2(\pi \nu/2) \ge 2(1-\nu)^2$ . **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 implies that

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

and

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

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

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

then  $\phi$  is continuous on the one-point compactification  $[0, \infty]$  of the closed halfline  $[0, \infty)$ . 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  $0 \le s \le \infty$  and  $0 \le X < \infty$ , 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), so  $|1 + X\phi(s)|^2 \ge [X\Im\phi(s)]^2 > 0$  for  $0 \le s < \infty$  and  $0 < X < \infty$ . Moreover,  $|1 + X\phi(\infty)|^2 \ge 1$  because  $\phi(\infty)$  is real and positive, and f(s,0) = 1 for  $0 \le s \le \infty$ . Finally, (40) and (41) imply that  $f(s,\infty) = |\phi(s)|^2 > 0$  for  $0 \le s \le \infty$ .

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

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

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  $a = \mu s^{-\nu} e^{\mp i \pi \nu}$  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 $s \rightarrow 0$ ,

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

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

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

*Proof.* From (37) and Lemma 10, 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 and 9,

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

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

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

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.

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

$$f'(x) > 0$$
 for  $0 < x < x^*$  and  $f'(x) < 0$  for  $x^* < x < 1$ , (42)

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

**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.  $\Box$ 

**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  $0 . Making the substitution <math>x = s^{\nu}$ , 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  $\alpha_-$ . 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 and sending  $\epsilon \to 0^+$  and  $R \to \infty$ , we conclude that

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

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

$$\lim_{z=\alpha_{\pm}} f(z) = \lim_{z \to \alpha_{\pm}} \left. \frac{d}{dz} (z - \alpha_{\pm})^2 f(z) = \frac{d}{dz} \left. \frac{(1 - pz)z^{1/\nu}}{(z - \alpha_{\mp})^2} \right|_{z=\alpha_{\pm}} = \mp i \frac{1 - \nu}{\nu} \frac{e^{i\pi/\nu}}{4q}$$

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 4, 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

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

Proof. By Lemma 11,

$$\mu B_1(s) + \mu^2 B_2(s) = s \left( \mu s^{-\nu} \cos \pi \nu + (\mu s^{-\nu})^2 + O(\mu + \mu^2 s^{-\nu}) \right) \text{ as } s \to 0^+,$$
  
and  $\mu B_1(s) + \mu^2 B_2(s) = O(\mu s^{-\nu} + \mu^2 s^{-2\nu}) \text{ as } s \to \infty, \text{ so } (37) \text{ implies that}$ 

$$\begin{aligned} |\delta^{n}(\mu)| &= \left| \frac{\sin \pi\nu}{\pi} \int_{0}^{\infty} e^{-ns} \mu s^{-\nu} \frac{\mu B_{1}(s) + \mu^{2} B_{2}(s)}{|1 + \mu s^{-\nu} e^{i\pi\nu}|^{2} |1 + \mu \psi_{+}(s)|^{2}} \frac{ds}{s} \right| \\ &\leq \frac{\sin \pi\nu}{\pi} \left( |I_{1}| + C_{\nu} I_{2} + C_{\nu} I_{3} \right), \end{aligned}$$

where, using Lemmas 8 and 9,

$$I_1 = \int_0^1 e^{-ns} \mu s^{-\nu} \frac{\mu s^{-\nu} \cos \pi \nu + (\mu s^{-\nu})^2}{|1 + \mu s^{-\nu} e^{i\pi\nu}|^2 |1 + \mu \psi_+(s)|^2} \, ds,$$
  
$$I_2 = \int_0^1 e^{-ns} \mu s^{-\nu} \frac{\mu + \mu^2 s^{-\nu}}{(1 + \mu^2 s^{-2\nu})^2} \, ds, \quad I_3 = \int_1^\infty e^{-ns} \mu s^{-\nu} \frac{\mu s^{-\nu} + \mu^2 s^{-2\nu}}{(1 + \mu^2 s^{-2\nu})^2} \, \frac{ds}{s}$$

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

$$n^{1+\nu}\rho^{-1}I_{2} \leq C\rho^{-2} \int_{0}^{\rho^{1/\nu}} e^{-s}s^{2\nu} \, ds + C\rho \int_{\rho^{1/\nu}}^{n} e^{-s}s^{-\nu} \, ds$$
$$\leq C \int_{0}^{\rho^{1/\nu}} e^{-s} \, ds + C\rho \int_{\rho^{1/\nu}}^{1} s^{-\nu} \, ds + C\rho \int_{1}^{\infty} e^{-s} \, ds$$
$$\leq C\rho^{1/\nu} + C(1-\nu)^{-1}\rho + C\rho \leq C(1-\nu)^{-1}\rho + C\rho^{1/\nu} \leq C_{\nu}\rho,$$

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

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

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  $q(x) < \min(2x^2, x^{-2} \cos \pi \nu + x^{-1})$  we have

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

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

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

Applying Lemma 13 with  $x = \rho^{1/\nu}$  and noting that  $1/\nu > 2$ , it follows that  $\int_0^n e^{-s}g(\rho s^{-\nu}) ds \leq C(\rho^{1/\nu} + \rho^2)$  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

 $I_1 \leq C_{\nu} n^{-1} \rho^2$ . Thus, assume now that  $1/2 < \nu < 1$  and note  $\cos \pi \nu < 0$ . Since

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

and, by Lemma 15,

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

we have

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

where

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

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

$$J_{3} = \int_{0}^{1} \left( |1+\mu s^{-\nu} e^{i\pi\nu}|^{2} - |1+\mu\psi_{+}(s)|^{2} \right) \frac{(\mu s^{-\nu})^{2} |\cos \pi\nu| + (\mu s^{-\nu})^{3}}{(1+\mu^{2}s^{-2\nu})^{3}} ds.$$

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

$$J_{1} \leq Cn^{-1}\rho^{1/\nu} \int_{n\rho^{-1/\nu}}^{\infty} \left( (2\nu - 1)s^{-2\nu} + s^{-3\nu} \right) ds$$
  
$$\leq Cn^{-1}\rho^{1/\nu} \left[ (n\rho^{-1/\nu})^{1-2\nu} + (n\rho^{-1/\nu})^{1-3\nu} \right]$$
  
$$= Cn^{-2\nu}\rho^{2} + Cn^{-3\nu}\rho^{3} \leq Cn^{-1}\rho^{2}.$$

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

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

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

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

and thus

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

Third, by Lemmas 10 and 11,

$$J_{3} \leq \int_{0}^{1} \left(\mu s^{1-\nu} + \mu^{2} s^{1-2\mu}\right) \frac{(\mu s^{-\nu})^{2} + (\mu s^{-\nu})^{3}}{(1+\mu s^{-\nu})^{3}} ds$$
$$= \mu^{1+1/\nu} \int_{0}^{\mu^{-1/\nu}} \frac{s(s^{-\nu} + s^{-2\nu})(s^{-2\nu} + s^{-3\nu})}{(1+s^{-2\nu})^{3}} ds$$
$$\leq (\rho n^{-\nu})^{1+1/\nu} \left(\int_{0}^{1} s^{1+\nu} ds + \int_{1}^{n\rho^{-1/\nu}} s^{1-3\nu} ds\right)$$

and applying Lemma 14 with  $x = n\rho^{-1/\nu}$  gives  $\int_{1}^{n\rho^{-1/\nu}} s^{1-3\nu} ds \leq 3(n\rho^{-1/\nu})^{1-\nu}$ so  $J_3 \leq Cn^{-\nu-1}\rho^{1+1/\nu}(1+n^{1-\nu}\rho^{1-1/\nu}) \leq C(n^{-\nu-1}\rho^{1+1/\nu}+n^{-2\nu}\rho^2) \leq Cn^{-1}\rho^2$ . Inserting the foregoing estimates for  $J_1$ ,  $J_2$  and  $J_3$  into (43) gives the desired estimate  $|I_1| \leq Cn^{-1}\rho^2$ , 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  $0 < t \le 1$ . 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  $m = 1, 2, 3, \dots$ 

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

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

but if  $r \ge 1/4$  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: 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).

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,

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

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,

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

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  $\alpha$ .



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

$$\Phi_{1}(\nu) = \sup_{0 < \mu < \infty} \max_{n^{\nu} \le \mu^{-1}} n^{1-2\nu} \mu^{-2} \delta^{n}(\mu), 
\Phi_{2}(\nu) = \sup_{0 < \mu < \infty} \sup_{n^{\nu} > \mu^{-1}} n^{1+\nu} \mu \delta^{n}(\mu),$$
(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 resticting n to the range  $1 \leq n \leq 200$ . We solved (12) and (16) 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  $\nu$  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  $\nu$ .

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