

A fitted scheme for a Caputo initial-boundary value problem

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Abstract In this paper we consider an initial-boundary value problem with a Caputo time derivative of order $\alpha \in (0, 1)$. The solution typically exhibits a weak singularity near the initial time and this causes a reduction in the orders of convergence of standard schemes. To deal with this singularity, the solution is computed with a fitted difference scheme on a graded mesh. The convergence of this scheme is analysed using a discrete maximum principle and carefully chosen barrier functions. Sharp error estimates are proved, which show an enhancement in the convergence rate compared with the standard L1 approximation on uniform meshes, and also indicate an optimal choice for the mesh grading. This optimal mesh grading is less severe than the optimal grading for the standard L1 scheme. Furthermore, the dependence of the error on the final time forms part of our error estimate. Numerical experiments are presented which corroborate our theoretical results.

Keywords Fractional differential equation · Caputo derivative · Weak singularity · Fitted scheme · Graded mesh

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1 Introduction

Mathematical models incorporating fractional differential equations arise in many branches of science and engineering (see [5, 12] and the references therein). Hence, it is no surprise that the design and analysis of appropriate numerical methods for solving such fractional differential equations has become a topical research area within the scientific computing community. In the present paper, we present a new numerical method for solving an initial-boundary value problem with a Caputo time-fractional derivative of order $\alpha \in (0, 1)$.

We shall consider the problem

$$(D_t^\alpha + \mathcal{L})u(x, t) = f(x, t) \quad (1a)$$

for $(x, t) \in Q := (0, l) \times (0, T]$, with

$$\mathcal{L}u := -p \frac{\partial^2 u}{\partial x^2} + c(x)u, \quad (1b)$$

and initial-boundary conditions

$$u(0, t) = u(l, t) = 0 \text{ for } t \in (0, T], \quad (1c)$$

$$u(x, 0) = \phi(x) \text{ for } x \in [0, l], \quad (1d)$$

where $0 < \alpha < 1$, p is a positive constant, $c \in C[0, l]$ with $c \geq 0$, $f \in C(\bar{Q})$ where $\bar{Q} := [0, l] \times [0, T]$, and $\phi \in C[0, l]$. Assume the compatibility conditions

$$\phi(0) = \phi(l) = 0 \quad (1e)$$

at the corners $(0, 0)$ and $(0, l)$ of \bar{Q} ; in Section 2 more regularity conditions will be imposed on the data of the problem. We consider homogeneous boundary conditions in problem (1) without loss of generality.

The Caputo fractional derivative [4] of order α with $0 < \alpha < 1$ is

$$D_t^\alpha \omega(x, t) := \frac{1}{\Gamma(1 - \alpha)} \int_{s=0}^t (t - s)^{-\alpha} \frac{\partial \omega(x, s)}{\partial s} ds \quad \text{for } 0 \leq x \leq l, 0 < t \leq T. \quad (2)$$

Typical solutions $u(x, t)$ of problem (1) exhibit an initial layer at $t = 0$ but nonetheless this singular behaviour has been considered in relatively few papers, e.g., [2, 9, 10, 13, 14, 18]. For each fixed x , the difference $u(x, t) - \phi(x)$ behaves like a multiple of t^α and consequently the time derivatives of u blow up as $t \rightarrow 0$.

In [18] the convergence in the discrete maximum norm of a standard finite difference scheme is analysed while taking into account this singular behaviour of u . The scheme uses the standard L1 approximation for $D_t^\alpha u$ on a graded temporal mesh and a standard finite difference approximation for $\mathcal{L}u$ on a uniform spatial mesh. It is proved that the method converges with order $O(M^{-2} + N^{-\min\{2-\alpha, r\alpha\}})$ where M and N are the spatial and temporal

discretization parameters and $r \geq 1$ is the mesh grading; the value of $r = 1$ corresponds to a uniform mesh and the larger r is, the more the grid condenses at $t = 0$. This error estimate is sharp and implies that one has to take $r \geq (2 - \alpha)/\alpha$ to yield the optimal order of convergence $O(M^{-2} + N^{-(2-\alpha)})$ method. Thus if α is close to zero, then the mesh will be very fine near $t = 0$ and in practice this could cause some difficulties with rounding error.

In the present paper we construct and analyse a new finite difference scheme that needs less severe grading of the optimal mesh. This scheme is designed to reflect the singular behaviour of the solution near $t = 0$: it constructs a difference approximation that is exact for the functions 1 and t^α , i.e., it is *fitted*. We shall prove error estimates for this fitted scheme showing that it is more accurate than the L1 scheme when applied to problems having the initial singularity described earlier.

A related idea was used implicitly in [10] but the finite element method there is more complicated than ours to implement, and an $L^\infty(L^2)$ -error bound is proved in [10] while our error bounds are in the stronger $L^\infty(L^\infty)$ -norm. See Remark 4 for more information.

The analysis of convergence of our fitted scheme is based on a decomposition of $u - \phi$ into a leading term that is $O(t^\alpha)$ as $t \rightarrow 0$ and a smoother remainder v (defined in Lemma 1). We shall combine truncation error estimates with a novel stability analysis based on a discrete maximum principle and appropriate barrier functions, obtaining sharp error estimates.

Similarly to [1], our discrete maximum principle is proved by means of an alternative definition of the Caputo fractional derivative (see [1, 19, 20]):

$$D_t^\alpha \omega(x, t) := \frac{1}{\Gamma(1 - \alpha)} \left\{ \frac{\omega(x, t) - \omega(x, 0)}{t^\alpha} + \alpha \int_{s=0}^t (t - s)^{-\alpha-1} [\omega(x, t) - \omega(x, s)] ds \right\} \quad (3)$$

for $0 \leq x \leq l$, $0 < t \leq T$. For all functions considered in the current paper the formulas (2) and (3) are equivalent, as can be seen from the conditions for this equivalence that are derived in [19, 20].

The alternative formulation (3) is helpful in (i) constructing finite-element type approximations of D_t^α such as our fitted approximation, (ii) giving a truncation error analysis that is different from the analysis in [18], and (iii) facilitating the use of discrete barrier functions in our analysis.

Our error estimates show that in the discrete maximum norm the fitted scheme has convergence rate $O(M^{-2} + N^{-\min\{2-\alpha, 2r\alpha\}})$ (which is an improvement on the rate reported above for [18]). It follows that the optimal choice of mesh grading for the fitted scheme is $r = \max\{1, (2 - \alpha)/(2\alpha)\}$. As well as this theoretical result, it is shown experimentally that the fitted scheme performs better than the standard L1 scheme on (i) uniform meshes (i.e., $r = 1$) and (ii) graded meshes with the optimal choice of the mesh grading for each scheme.

The superiority of the fitted scheme for $r = 1$ is apparent from the theoretical convergence rates. On optimally graded meshes for both schemes, the

fitted scheme has smaller errors because it requires less mesh grading and consequently its mesh is not as severely clustered near $t = 0$.

In some applications, large values of the terminal time T are used. Thus it is of interest to explore how error bounds depend on T , and our analysis of the fitted scheme will do this. Numerical results will demonstrate the sharpness of our theoretical error bound as a function of T .

The structure of the paper is as follows. In Section 2 we establish the decomposition of u that will be used to analyse the convergence of the fitted scheme. Estimates for the derivatives of the remainder v near $t = 0$ and for large t are given. The fitted scheme is constructed in Section 3 on a general graded mesh. The convergence of this scheme is analysed in Section 4 and we give our main convergence result where error estimates are proved in the discrete maximum norm. Numerical results in Section 5 for the L1 and fitted schemes show that the fitted scheme is more accurate than the L1 scheme. In addition, they corroborate the sharpness of our error estimates regarding both the orders of convergence and the dependence of the error on the final time T .

Notation: We use the standard Hilbert space $L_2(0, l)$ with norm $\|\cdot\|_2$ and inner product (\cdot, \cdot) . In this paper C denotes a generic constant that depends on the data of the boundary value problem (1) but is independent of T and of any mesh used to solve (1) numerically; note that C can take different values in different places.

2 Decomposition of the continuous solution

This section gives a decomposition of the solution u of (1) that will be used to analyse the convergence of the fitted scheme. The regularity of u is discussed in [18, Section 2] and it is shown in [18, Theorem 2.1] that

$$\left| \frac{\partial^k u}{\partial x^k}(x, t) \right| \leq C \quad \text{for } k = 0, 1, 2, 3, 4, \quad (4a)$$

$$\left| \frac{\partial^\ell u}{\partial t^\ell}(x, t) \right| \leq C(1 + t^{\alpha-\ell}) \quad \text{for } \ell = 0, 1, 2, \quad (4b)$$

for all $(x, t) \in [0, l] \times (0, T]$, under some regularity conditions on the data problem.

Set

$$g(x, t) = f(x, t) - f(x, 0) + \frac{\mathcal{L}(\mathcal{L}\phi(x) - f(x, 0))}{\Gamma(1 + \alpha)} t^\alpha \quad \text{for } (x, t) \in Q.$$

Lemma 1 *Assume that $\phi \in C^4[0, l]$, $c \in C^2[0, l]$ and $f, f_x, f_{xx} \in C(\bar{Q})$. Assume also that $f(0, 0) = f(l, 0) = 0$ and $\phi''(0) = \phi''(l) = 0$. Then the solution of the problem (1) can be decomposed as*

$$u(x, t) = \phi(x) + \frac{f(x, 0) - \mathcal{L}\phi(x)}{\Gamma(1 + \alpha)} t^\alpha + v(x, t) \quad (5)$$

where the remainder term $v(x, t)$ is the solution of the following problem:

$$(D_t^\alpha + \mathcal{L})v(x, t) = g(x, t) \text{ for } (x, t) \in Q,$$

with initial-boundary conditions

$$v(0, t) = v(l, t) = 0 \text{ for } t \in (0, T], \quad v(x, 0) = 0 \text{ for } x \in [0, l].$$

Proof Define

$$v(x, t) := u(x, t) - \phi(x) + \frac{\mathcal{L}\phi(x) - f(x, 0)}{\Gamma(1 + \alpha)} t^\alpha \text{ for } (x, t) \in \bar{Q}.$$

Then (5) is satisfied, and $v(0, t) = v(l, t) = 0$ for $t \in (0, T]$ follows from (1c), (1e) and our hypotheses on f and ϕ'' . Next, $v(x, 0) = 0$ for $x \in [0, l]$ is immediate from (1d). Finally, from (1a) and $D_t^\alpha t^\alpha = \Gamma(1 + \alpha)$ we get

$$(D_t^\alpha + \mathcal{L})v(x, t) = f(x, t) - \mathcal{L}\phi(x) - [f(x, 0) - \mathcal{L}\phi(x)] + \frac{\mathcal{L}(\mathcal{L}\phi(x) - f(x, 0))}{\Gamma(1 + \alpha)} t^\alpha,$$

as desired.

Remark 1 The decomposition (5) can be motivated as follows. Suppose that

$$u(x, t) = \phi(x) + z(x)t^\alpha + v(x, t) \tag{6}$$

for some function v whose time derivatives are smoother than those of u ; this is a reasonable assumption since we know from [18] that for each x , $u(x, t) - \phi(x)$ behaves like a multiple of t^α . Now the argument of [17] shows that for each fixed x ,

$$D_t^\alpha v(x, t) \rightarrow 0 \text{ as } t \rightarrow 0.$$

Consequently, substituting (6) into (1a) then letting t go to zero, one gets

$$\mathcal{L}\phi(x) + z(x)\Gamma(1 + \alpha) = f(x, 0),$$

since $v(x, 0) \equiv 0$ and hence $\mathcal{L}v(x, 0) \equiv 0$. Solving this equation for $z(x)$ then substituting into (6) yields (5).

Remark 2 The decomposition (5) and $|u(x, t)| \leq C$ (from (4a)) for $(x, t) \in \bar{Q}$ show that the remainder v satisfies

$$|v(x, t)| = \left| u(x, t) - \phi(x) - \frac{f(x, 0) - \mathcal{L}\phi(x)}{\Gamma(1 + \alpha)} t^\alpha \right| \leq C(1 + t^\alpha).$$

Observe that if u is bounded as $t \rightarrow \infty$, then v must blow up like t^α as $t \rightarrow \infty$ to ensure that (5) is valid. Nevertheless, in Theorem 3 we shall see that v_t and v_{tt} are bounded as $t \rightarrow \infty$.

The rest of this section is devoted to proving bounds on the remainder v . To derive these we use separation of variables and a regularity framework similar to [16]. Thus let $\{(\lambda_i, \psi_i) : i = 1, 2, \dots\}$ be the eigenvalues and eigenfunctions for the Sturm-Liouville two-point boundary value problem

$$\mathcal{L}\psi_i = -p\psi_i'' + c\psi_i = \lambda_i\psi_i \text{ on } (0, l), \quad \psi_i(0) = \psi_i(l) = 0. \quad (7)$$

The eigenfunctions are normalised by requiring $\|\psi_i\|_2 = 1$ for all i and it is well known that $\lambda_i > 0$ for all i .

Set

$$D(\mathcal{L}^\gamma) = \left\{ \omega \in L_2(0, l) : \sum_{i=1}^{\infty} \lambda_i^{2\gamma} |(\omega, \psi_i)|^2 < \infty \right\} \text{ for } \gamma \geq 0,$$

the domain of the fractional power \mathcal{L}^γ of the operator \mathcal{L} (see [8, 16]). Also set

$$\|\omega\|_{\mathcal{L}^\gamma} = \left(\sum_{i=1}^{\infty} \lambda_i^{2\gamma} |(\omega, \psi_i)|^2 \right)^{1/2}$$

and $\omega_i(t) := (\omega(\cdot, t), \psi_i(\cdot))$ for $i = 1, 2, \dots$

In this framework the bounds (4) are proved in [18, Theorem 2.1] under the hypotheses that

$$\phi \in D(\mathcal{L}^{5/2}), f(\cdot, t) \in D(\mathcal{L}^{5/2}), f_t(\cdot, t) \text{ and } f_{tt}(\cdot, t) \in D(\mathcal{L}^{1/2}) \quad (8a)$$

for each $t \in (0, T]$, and

$$\|f(\cdot, t)\|_{\mathcal{L}^{5/2}} + \|f_t(\cdot, t)\|_{\mathcal{L}^{1/2}} + \min\{1, t^\rho\} \|f_{tt}(\cdot, t)\|_{\mathcal{L}^{1/2}} \leq C \quad (8b)$$

for all $t \in (0, T]$ and some constant $0 < \rho < 1$, where C is a constant independent of t . In the present paper we assume that the regularity conditions (8a) and (8b) are satisfied, and that

$$f_{ttt}(\cdot, t) \in D(\mathcal{L}^{1/2}), \quad (8c)$$

$$\|f_t(\cdot, t)\|_{\mathcal{L}^{1/2}} + \|f_{tt}(\cdot, t)\|_{\mathcal{L}^{1/2}} + \min\{1, t^\rho\} \|f_{ttt}(\cdot, t)\|_{\mathcal{L}^{1/2}} \leq C, \quad (8d)$$

for all $t \in (0, T]$, where ρ and C are constants independent of t with $0 < \rho < 1$.

The following calculation appears a few times in our analysis. Suppose that $\omega(\cdot, s) \in D(\mathcal{L}^{1/2})$ and $\|\omega(\cdot, s)\|_{\mathcal{L}^{1/2}} \leq C$ for $0 \leq s \leq T$. Then

$$\sum_{i=1}^{\infty} |\omega_i(s)| \leq \left(\sum_{i=1}^{\infty} \frac{1}{\lambda_i} \right)^{1/2} \left(\sum_{i=1}^{\infty} \lambda_i \omega_i^2(s) \right)^{1/2} \leq C \|\omega\|_{\mathcal{L}^{1/2}} \quad \text{for } 0 \leq s \leq t, \quad (9)$$

from a Cauchy-Schwarz inequality and $\lambda_i \approx i^2$ [3, p.335].

Theorems 1 and 3 establish bounds on the derivatives of the remainder v for $t \leq 1$ and $t > 1$, respectively. Their proofs require the generalized Mittag-Leffler function [15], which is defined by

$$E_{\gamma, \delta}(r) := \sum_{k=0}^{\infty} \frac{r^k}{\Gamma(\gamma k + \delta)} \text{ for } \gamma > 0, \delta \in \mathbb{R} \text{ and } r \in \mathbb{R}.$$

One has [15, Theorem 1.6]

$$|E_{\gamma,\delta}(-r)| \leq \frac{C}{1+r} \leq C \text{ for } 0 < \gamma < 2, \delta \in \mathbb{R}, \text{ and all } r \geq 0. \quad (10)$$

Theorem 1 *Assume the hypotheses of Lemma 1 and (8). Then there exists a constant C such that for all $(x, t) \in [0, l] \times (0, 1]$ one has*

$$\left| \frac{\partial^\ell v}{\partial t^\ell}(x, t) \right| \leq Ct^{2\alpha-\ell} \text{ for } \ell = 0, 1, 2.$$

Proof We imitate the argument in [18, Section 2]. A standard separation of variables technique yields

$$v(x, t) = \sum_{i=1}^{\infty} \left[\int_{s=0}^t s^{\alpha-1} E_{\alpha,\alpha}(-\lambda_i s^\alpha) g_i(t-s) ds \right] \psi_i(x),$$

where $g_i(t) = (g(\cdot, t), \psi_i(\cdot))$; cf. [18, (2.2)] and recall that $v(x, 0) = 0$ for $x \in [0, l]$.

To estimate v_t and v_{tt} write $v = v^{(1)} + v^{(2)}$, where

$$v^{(1)}(x, t) := \sum_{i=1}^{\infty} \left[\int_{s=0}^t s^{\alpha-1} E_{\alpha,\alpha}(-\lambda_i s^\alpha) [f_i(t-s) - f_i(0)] ds \right] \psi_i(x), \quad (11)$$

$$v^{(2)}(x, t) := \sum_{i=1}^{\infty} \left[(\mathcal{L}(\mathcal{L}\phi(x) - f(x, 0)), \psi_i(x)) \right. \\ \left. \times \frac{1}{\Gamma(1+\alpha)} \int_{s=0}^t s^{\alpha-1} E_{\alpha,\alpha}(-\lambda_i s^\alpha) (t-s)^\alpha ds \right] \psi_i(x). \quad (12)$$

The correctness of this decomposition can be seen easily by inspecting Lemma 1.

First, consider $v^{(1)}$. Integrating (11) by parts and using [7, (4.3.1)] yields

$$v^{(1)}(x, t) = \sum_{i=1}^{\infty} \left[\int_{s=0}^t s^\alpha E_{\alpha,1+\alpha}(-\lambda_i s^\alpha) f'_i(t-s) ds \right] \psi_i(x). \quad (13)$$

Recalling (10) and using (9) and the hypothesis $f_t \in D(\mathcal{L}^{1/2})$ from (8d) gives

$$\int_{s=0}^t s^\alpha \sum_{i=1}^{\infty} |f'_i(t-s)| ds \leq C \int_{s=0}^t s^\alpha ds \leq Ct^{\alpha+1}. \quad (14)$$

Thus

$$|v^{(1)}(x, t)| \leq \sum_{i=1}^{\infty} \left[\int_{s=0}^t s^\alpha E_{\alpha,1+\alpha}(-\lambda_i s^\alpha) |f'_i(t-s)| ds \right] \leq C, \quad (15)$$

using $|\psi_i(x)| \leq C$ for all i and x [3, p.335], (10) and (14).

We now consider $v_t^{(1)}$. Differentiate (13) term-by-term with respect to t for $(x, t) \in Q$ and again use $|\psi_i(x)| \leq C$ and (10) to get

$$\begin{aligned} & \left| \sum_{i=1}^{\infty} \left[t^\alpha E_{\alpha, 1+\alpha}(-\lambda_i t^\alpha) f_i'(0) + \int_{s=0}^t s^\alpha E_{\alpha, 1+\alpha}(-\lambda_i s^\alpha) f_i''(t-s) ds \right] \psi_i(x) \right| \\ & \leq C t^\alpha \sum_{i=1}^{\infty} |f_i'(0)| + C \sum_{i=1}^{\infty} \int_{s=0}^t s^\alpha |f_i''(t-s)| ds \\ & \leq C t^\alpha, \end{aligned} \quad (16)$$

where the f_i terms are bounded as in (14). Thus for each fixed $t \in [0, 1]$, the series in (16) is absolutely and uniformly convergent for $(x, t) \in [0, l] \times [0, 1]$, so it equals $v_t^{(1)}(x, t)$ on $[0, l] \times [0, 1]$ and we obtain

$$|v_t^{(1)}(x, t)| \leq C t^\alpha, \text{ for } (x, t) \in [0, l] \times [0, 1]. \quad (17)$$

Next, we bound $v_{tt}^{(1)}$. Differentiating (13) twice term-by-term with respect to t and using [7, (4.3.1)], (10) and $|\psi_i(x)| \leq C$ yields

$$\begin{aligned} & \left| \sum_{i=1}^{\infty} \left[t^{\alpha-1} E_{\alpha, \alpha}(-\lambda_i t^\alpha) f_i'(0) + t^\alpha E_{\alpha, 1+\alpha}(-\lambda_i t^\alpha) f_i''(0) \right. \right. \\ & \quad \left. \left. + \int_{s=0}^t s^\alpha E_{\alpha, 1+\alpha}(-\lambda_i s^\alpha) f_i'''(t-s) ds \right] \psi_i(x) \right| \\ & \leq C t^{\alpha-1} \sum_{i=1}^{\infty} |f_i'(0)| + C t^\alpha \sum_{i=1}^{\infty} |f_i''(0)| + C \sum_{i=1}^{\infty} \int_{s=0}^t s^\alpha |f_i'''(t-s)| ds \end{aligned} \quad (18)$$

for $(x, t) \in [0, l] \times (0, 1]$. The bounds

$$\sum_{i=1}^{\infty} |f_i'(0)| \leq C \text{ and } \sum_{i=1}^{\infty} |f_i''(0)| \leq C \quad (19)$$

for the first two sums in (18) are obtained by applying (9). It remains to bound the final sum in (18). From (8d) and (9) one has

$$\sum_{i=1}^{\infty} |f_i'''(t-s)| \leq C(t-s)^{-\rho}.$$

Hence

$$\int_{s=0}^t s^\alpha \sum_{i=1}^{\infty} |f_i'''(t-s)| ds \leq C \int_{s=0}^t s^\alpha (t-s)^{-\rho} ds \leq C t^{\alpha+(1-\rho)} \quad (20)$$

from a standard identity [4, Theorem D.6] for the Euler Beta function. Now use (19) and (20) in (18) to get

$$\begin{aligned} & \left| \sum_{i=1}^{\infty} [t^{\alpha-1} E_{\alpha,\alpha}(-\lambda_i t^\alpha) f_i'(0) + t^\alpha E_{\alpha,1+\alpha}(-\lambda_i t^\alpha) f_i''(0) \right. \\ & \quad \left. + \int_{s=0}^t s^\alpha E_{\alpha,1+\alpha}(-\lambda_i s^\alpha) f_i'''(t-s) ds \right] \psi_i(x) \Big| \\ & \leq C t^{\alpha-1} + C t^\alpha + C t^{\alpha+(1-\rho)}. \end{aligned} \quad (21)$$

Thus the series in (21) is absolutely and uniformly convergent for $(x, t) \in [0, l] \times [\varepsilon, t]$ for each $\varepsilon \in (0, t]$, so it equals $v_{tt}^{(1)}$ on $[0, l] \times (0, 1]$ and one has

$$|v_{tt}^{(1)}(x, t)| \leq C(t^{\alpha-1} + t^\alpha + t^{\alpha+(1-\rho)}) \leq C t^{\alpha-1}. \quad (22)$$

We now consider $v^{(2)}$. From (12) and [15, (1.100)],

$$v^{(2)}(x, t) = \sum_{i=1}^{\infty} [t^{2\alpha} (\mathcal{L}(\mathcal{L}\phi(x) - f(x, 0)), \psi_i) E_{\alpha,1+2\alpha}(-\lambda_i t^\alpha)] \psi_i(x). \quad (23)$$

Using $|\psi_i(x)| \leq C$ and (10) gives

$$\begin{aligned} |v^{(2)}(x, t)| & \leq C t^{2\alpha} \sum_{i=1}^{\infty} |(\mathcal{L}(\mathcal{L}\phi(x) - f(x, 0)), \psi_i)| \\ & = C t^{2\alpha} \sum_{i=1}^{\infty} |(\mathcal{L}\phi(x) - f(x, 0), \mathcal{L}\psi_i)| \end{aligned} \quad (24)$$

on integrating by parts and using $\phi(0) = \phi(l) = 0$, $\phi''(0) = \phi''(l) = 0$ and $f(0, 0) = f(l, 0) = 0$. The series in (24) satisfies

$$\begin{aligned} \sum_{i=1}^{\infty} |(\mathcal{L}\phi(x) - f(x, 0), \mathcal{L}\psi_i)| & = \sum_{i=1}^{\infty} \lambda_i |(\mathcal{L}\phi(x) - f(x, 0), \psi_i)| \\ & = \sum_{i=1}^{\infty} \lambda_i |[(\phi(x), \mathcal{L}\psi_i) - (f(x, 0), \psi_i)]| \\ & = \sum_{i=1}^{\infty} \lambda_i |[\lambda_i (\phi(x), \psi_i) - (f(x, 0), \psi_i)]|, \end{aligned}$$

as (λ_i, ψ_i) are an eigenpair of (7). Now use $\phi \in D(\mathcal{L}^{5/2})$, $f(\cdot, t) \in D(\mathcal{L}^{3/2})$ (as $f(\cdot, t) \in D(\mathcal{L}^{5/2})$) and $\|f(\cdot, t)\|_{\mathcal{L}^{3/2}} \leq C$ in a calculation resembling (14), to obtain

$$\sum_{i=1}^{\infty} |(\mathcal{L}(\mathcal{L}\phi(x) - f(x, 0)), \psi_i)| \leq C. \quad (25)$$

From (24) and (25), we have

$$|v^{(2)}(x, t)| \leq C t^{2\alpha}. \quad (26)$$

Differentiating (23) term-by-term with respect to t , from [7, (4.3.1)], (10) and $|\psi_i(x)| \leq C$ one can prove that for $\ell = 1, 2$ one has

$$\begin{aligned} & \sum_{i=1}^{\infty} \left| \frac{\partial^\ell}{\partial t^\ell} (t^{2\alpha} [(\mathcal{L}(\mathcal{L}\phi(x) - f(x, 0)), \psi_i) E_{\alpha, 1+2\alpha}(-\lambda_i t^\alpha)] \psi_i(x)) \right| \\ &= \sum_{i=1}^{\infty} \left| (t^{2\alpha-\ell} [(\mathcal{L}(\mathcal{L}\phi(x) - f(x, 0)), \psi_i) E_{\alpha, 1+2\alpha-\ell}(-\lambda_i t^\alpha)] \psi_i(x)) \right| \\ &\leq C t^{2\alpha-\ell} \sum_{i=1}^{\infty} |(\mathcal{L}(\mathcal{L}\phi(x) - f(x, 0)), \psi_i)| \\ &\leq C t^{2\alpha-\ell}, \end{aligned} \quad (27)$$

where we have used (25) in the last inequality. Thus the series in (27) is absolutely and uniformly convergent for $(x, t) \in [0, l] \times [\varepsilon, 1]$ for each $\varepsilon \in (0, 1]$, so it equals $v_t^{(2)}$ and $v_{tt}^{(2)}$ on Q for $\ell = 1, 2$ respectively; consequently

$$\left| \frac{\partial^\ell v^{(2)}}{\partial t^\ell}(x, t) \right| \leq C t^{2\alpha-\ell} \text{ for } \ell = 1, 2 \text{ and } (x, t) \in Q. \quad (28)$$

Recall that $v = v^{(1)} + v^{(2)}$. Combining (15), (26), (17), (22) and (28), the theorem is proved.

A comparison of (4b) and Theorem 1 shows that v is better behaved than u near $t = 0$.

Next, the behaviour of u and v is analysed when $t > 1$. Some estimates for u are proved in Theorem 2 and are used to deduce bounds on v in Theorem 3.

We shall need a sharper estimate than (10) in the particular case when the two parameters of the Mittag-Leffler function are equal. From [15, (1.143)], one has

$$|E_{\gamma, \gamma}(-r)| \leq \frac{C}{1+r^2} \leq \frac{C}{r^2} \text{ for } 0 < \gamma < 2 \text{ and } r \geq 0. \quad (29)$$

Theorem 2 Assume (8) and $T > 1$. Then the solution u of (1) satisfies

$$\left| \frac{\partial^\ell u}{\partial t^\ell}(x, t) \right| \leq C, \text{ for } \ell = 1, 2 \text{ and } (x, t) \in [0, l] \times [1, T].$$

Proof In [11, (4.29)], [16, (2.11)] or [18, Section 2], the solution u to problem (1) is given by

$$u(x, t) = \sum_{i=1}^{\infty} \left[(\phi, \psi_i) E_{\alpha, 1}(-\lambda_i t^\alpha) + J_i(t) \right] \psi_i(x) \quad (30)$$

where

$$J_i(t) := \int_{s=0}^t s^{\alpha-1} E_{\alpha, \alpha}(-\lambda_i s^\alpha) f_i(t-s) ds \quad \text{with} \quad f_i(t) := (f(\cdot, t), \psi_i(\cdot)).$$

Differentiating term-by-term with respect to t for $(x, t) \in Q$ yields

$$\begin{aligned} & \sum_{i=1}^{\infty} \left[-(\phi, \psi_i) \lambda_i t^{\alpha-1} E_{\alpha, \alpha}(-\lambda_i t^\alpha) + t^{\alpha-1} E_{\alpha, \alpha}(-\lambda_i t^\alpha) f_i(0) \right. \\ & \quad \left. + \int_{s=0}^t s^{\alpha-1} E_{\alpha, \alpha}(-\lambda_i s^\alpha) f_i'(t-s) ds \right] \psi_i(x), \end{aligned} \quad (31)$$

where a standard formula [11, p.154, line 2] is used to differentiate $E_{\alpha, 1}(\cdot)$. We bound each term as in [18, Section 2], obtaining for the first two terms

$$\begin{aligned} & \sum_{i=1}^{\infty} |(\phi, \psi_i) \lambda_i t^{\alpha-1} E_{\alpha, \alpha}(-\lambda_i t^\alpha) \psi_i(x)| \leq C t^{\alpha-1} \leq C, \\ & \sum_{i=1}^{\infty} |t^{\alpha-1} E_{\alpha, \alpha}(-\lambda_i t^\alpha) f_i(0) \psi_i(x)| \leq C t^{\alpha-1} \leq C. \end{aligned}$$

Consider now the last term in (31). From (9) with $\omega = f_t(\cdot, t)$ and the estimate (29), we get

$$\begin{aligned} \int_{s=0}^t s^{\alpha-1} \sum_{i=1}^{\infty} E_{\alpha, \alpha}(-\lambda_i s^\alpha) |f_i'(t-s)| ds & \leq C \int_{s=0}^t \frac{s^{\alpha-1}}{1+s^{2\alpha}} \sum_{i=1}^{\infty} |f_i'(t-s)| ds \\ & \leq C \int_{s=0}^t \frac{s^{\alpha-1}}{1+s^{2\alpha}} ds \\ & \leq C \left(\int_{s=0}^1 s^{\alpha-1} ds + \int_{s=1}^t s^{-\alpha-1} ds \right) \\ & \leq C. \end{aligned}$$

Thus,

$$\left| \sum_{i=1}^{\infty} \left[\int_{s=0}^t s^{\alpha-1} E_{\alpha, \alpha}(-\lambda_i s^\alpha) f_i'(t-s) ds \right] \psi_i(x) \right| \leq C,$$

where we have used $|\psi_i| \leq C$.

From the previous estimates for the three terms in (31), we infer that this expression equals $u_t(x, t)$ and

$$\left| \frac{\partial u}{\partial t}(x, t) \right| \leq C \text{ for } (x, t) \in [0, l] \times [1, T].$$

A similar argument proves the theorem for the case $\ell = 2$.

Theorem 3 *Assume the hypothesis of Lemma 1 and (8). Assume that $T > 1$. Then*

$$\left| \frac{\partial^\ell v}{\partial t^\ell}(x, t) \right| \leq C, \quad \text{for } \ell = 1, 2 \text{ and } (x, t) \in [0, l] \times [1, T].$$

Proof This result follows from the decomposition (5) and Theorem 2.

3 The discretisation

We shall approximate the solution of problem (1) using a finite difference scheme on a mesh that is uniform in space and graded in time.

Let M and N be positive integers. Set $h = l/M$ and $x_m := mh$ for $m = 0, 1, \dots, M$. Set $t_n = T(n/N)^r$ for $n = 0, 1, \dots, N$ where the constant mesh grading $r \geq 1$ is chosen by the user. If $r = 1$, then the mesh is uniform. Set $\tau_n = t_n - t_{n-1}$ for $n = 1, 2, \dots, N$. Then

$$\tau_{n+1} = T \left(\frac{n+1}{N} \right)^r - T \left(\frac{n}{N} \right)^r \leq CTN^{-r} n^{r-1} = Cn^{-1}t_n \quad (32)$$

for $n = 0, 1, \dots, N-1$.

The mesh is $\{(x_m, t_n) : m = 0, 1, \dots, M, n = 0, 1, \dots, N\}$. The approximate solution computed at the mesh point (x_m, t_n) is denoted by u_m^n .

Our fitted scheme is inspired by the decomposition (5). We approximate $g(x, t) - g(x, s)$ in the Caputo derivative (3) by linear combinations of the functions $1, t^\alpha$ on each temporal subinterval. That is, for $0 \leq s \leq T$ consider the basis functions

$$\phi_0(s) = \begin{cases} \frac{t_1^\alpha - s^\alpha}{t_1^\alpha} & \text{for } 0 \leq s \leq t_1, \\ 0 & \text{otherwise,} \end{cases} \quad (33a)$$

$$\phi_k(s) = \begin{cases} \frac{s^\alpha - t_{k-1}^\alpha}{t_k^\alpha - t_{k-1}^\alpha} & \text{for } t_{k-1} \leq s \leq t_k, \\ \frac{t_{k+1}^\alpha - s^\alpha}{t_{k+1}^\alpha - t_k^\alpha} & \text{for } t_k \leq s \leq t_{k+1}, \\ 0 & \text{otherwise,} \end{cases} \quad \text{for } k = 1, 2, \dots, N-1, \quad (33b)$$

$$\phi_N(s) = \begin{cases} \frac{s^\alpha - t_{N-1}^\alpha}{t_N^\alpha - t_{N-1}^\alpha} & \text{for } t_{N-1} \leq s \leq t_N, \\ 0 & \text{otherwise.} \end{cases} \quad (33c)$$

It is straightforward to check that for $0 \leq s \leq t_n$ and any fixed x , the approximation $g(x, s) \approx \sum_{k=0}^n g(x, t_k) \phi_k(s)$ is exact for if $g(x, s)$ is constant or $g(x, s)$ is a multiple of t^s .

In general, for $0 \leq s \leq t_n$, write

$$g(x, t_n) - g(x, s) = g(x, t_n) \sum_{k=0}^n \phi_k(s) - g(x, s) \approx \sum_{k=0}^n \phi_k(s) [g(x, t_n) - g(x, t_k)].$$

Using this approximation in the Caputo fractional derivative formula (3), $D_t^\alpha u(x_m, t_n)$ is discretised by

$$\begin{aligned} D_N^\alpha u_m^n &:= \frac{1}{\Gamma(1-\alpha)} \left\{ \frac{u_m^n - u_m^0}{t_n^\alpha} \right. \\ &\quad \left. + \alpha \int_{s=0}^{t_n} (t_n - s)^{-\alpha-1} \left[\sum_{k=0}^{n-1} \phi_k(s) (u_m^n - u_m^k) \right] ds \right\} \\ &= \frac{1}{\Gamma(1-\alpha)} \left\{ \frac{u_m^n - u_m^0}{t_n^\alpha} \right. \\ &\quad \left. + \alpha (u_m^n - u_m^0) I_n^0 + \alpha \sum_{k=1}^{n-1} (u_m^n - u_m^k) (I_{nk}^- + I_{nk}^+) \right\}, \quad (34) \end{aligned}$$

where we used the definition (33) of the ϕ_k , and

$$\begin{aligned} I_n^0 &:= \int_{s=t_0}^{t_1} (t_n - s)^{-\alpha-1} \phi_0(s) ds \\ &= -\frac{t_n^{-\alpha}}{\alpha} + \frac{1}{t_1^\alpha} \int_{s=0}^{t_1} s^{\alpha-1} (t_n - s)^{-\alpha} ds, \\ I_{nk}^- &:= \int_{s=t_{k-1}}^{t_k} (t_n - s)^{-\alpha-1} \phi_k(s) ds \\ &= \frac{(t_n - t_k)^{-\alpha}}{\alpha} - \frac{1}{t_k^\alpha - t_{k-1}^\alpha} \int_{s=t_{k-1}}^{t_k} s^{\alpha-1} (t_n - s)^{-\alpha} ds, \\ I_{nk}^+ &:= \int_{s=t_k}^{t_{k+1}} (t_n - s)^{-\alpha-1} \phi_k(s) ds \\ &= -\frac{(t_n - t_k)^{-\alpha}}{\alpha} + \frac{1}{t_{k+1}^\alpha - t_k^\alpha} \int_{s=t_k}^{t_{k+1}} s^{\alpha-1} (t_n - s)^{-\alpha} ds. \end{aligned}$$

Here the integrations by parts are valid since the functions $(t_n - s)^{-\alpha} \phi_k(s)$ are absolutely continuous on $[t_{j-1}, t_j]$ for $j = 1, 2, \dots, n$ and $k = 0, 1, \dots, n-1$.

Substituting these three expressions into (34) and gathering terms, one obtains the following alternative formulation of (34):

$$D_N^\alpha u_m^n = \frac{\alpha}{\Gamma(1-\alpha)} \sum_{k=0}^{n-1} \frac{u_m^{k+1} - u_m^k}{t_{k+1}^\alpha - t_k^\alpha} \int_{s=t_k}^{t_{k+1}} s^{\alpha-1} (t_n - s)^{-\alpha} ds, \quad (35)$$

which can be recognised as an approximation of the formula (2) for $D_t^\alpha u(x_m, t_n)$.

The diffusion term in (1b) is approximated by a standard second-order discretisation:

$$u_{xx}(x_m, t_n) \approx \delta_x^2 u_m^n := \frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{h^2}.$$

Thus we approximate (1) by the discrete problem

$$L_{M,N}u_m^n := D_N^\alpha u_m^n - p \delta_x^2 u_m^n + c(x_m)u_m^n = f(x_m, t_n) \quad (36a)$$

$$\text{for } 1 \leq m \leq M-1, 1 \leq n \leq N;$$

$$u_0^n = u_M^n = 0 \text{ for } 0 < n \leq N, \quad (36b)$$

$$u_m^0 = \phi(x_m) \text{ for } 0 \leq m \leq M. \quad (36c)$$

Remark 3 In practice, the weights of the approximation (35) are computed from

$$\begin{aligned} \int_{s=t_k}^{t_{k+1}} s^{\alpha-1} (t_n - s)^{-\alpha} ds &= \int_{s=t_k/t_n}^{t_{k+1}/t_n} s^{\alpha-1} (1-s)^{-\alpha} ds \\ &= B(t_{k+1}/t_n; \alpha, 1-\alpha) - B(t_k/t_n; \alpha, 1-\alpha), \end{aligned}$$

where $B(z; \gamma, \delta)$ is the incomplete Beta function defined by

$$B(z; \gamma, \delta) := \int_{s=0}^z s^{\gamma-1} (1-s)^{\delta-1} ds \text{ for } \gamma, \delta > 0.$$

Remark 4 In [10] a method based on the L1 approximation and a proper orthogonal decomposition is used to approximate (1). It incorporates functions that are constructed to approximate the main singularity in the solution, as our method does. But a fundamental difference between the two approaches is that from the outset we include explicit basis functions that mimic the main singularity, while [10] starts with general basis functions then modifies them adaptively to approximate this singularity. Both approaches yield an error term that is $O(t^{2\alpha})$, though we work with $L^\infty(L^\infty)$ (see Theorem 4 below) while [10, Theorem 3.6] uses $L^\infty(L^2)$.

4 Convergence analysis of the difference scheme

The discretisation of the spatial derivative satisfies

$$\frac{\partial^2 u}{\partial x^2}(x_m, t_n) = \delta_x^2 u(x_m, t_n) + O(h^2). \quad (37)$$

Section 4.1 gives truncation error estimates for the discretisation (35) of the Caputo temporal derivative. In Section 4.2 we derive stability and error estimates for our fitted scheme.

4.1 Truncation error estimates for the temporal fractional derivative

Comparing the definition (3) of the Caputo fractional derivative and the derivation of its discretisation (34), one sees that the truncation error can

be written as follows:

$$\begin{aligned}
& (D_N^\alpha - D_t^\alpha)u(x_m, t_n) \\
&= \frac{\alpha}{\Gamma(1-\alpha)} \int_{s=0}^{t_n} (t_n - s)^{-\alpha-1} \left[u(x_m, s) - \sum_{k=0}^n \phi_k(s)u(x_m, t_k) \right] ds \\
&= \frac{\alpha}{\Gamma(1-\alpha)} \int_{s=0}^{t_n} (t_n - s)^{-\alpha-1} (u - \bar{u})(x_m, s) ds, \tag{38}
\end{aligned}$$

where \bar{u} denotes the fitted interpolant of any suitable function w :

$$\bar{w}(x_m, s) := \sum_{k=0}^n \phi_k(s)w(x_m, t_k) \text{ for } s \in [0, t_n].$$

We saw already that our temporal discretisation is exact for the functions 1 and t^α when x is fixed. It then follows from the decomposition (5) of u that

$$\begin{aligned}
(D_N^\alpha - D_t^\alpha)u(x_m, t_n) &= (D_N^\alpha - D_t^\alpha)v(x_m, t_n) \\
&= \frac{\alpha}{\Gamma(1-\alpha)} \int_{s=0}^{t_n} (t_n - s)^{-\alpha-1} (v - \bar{v})(x_m, s) ds. \tag{39a}
\end{aligned}$$

From (2), (33) and (35) one has the following equivalent representations for the truncation error, which will also be used in our analysis:

$$(D_N^\alpha - D_t^\alpha)v(x_m, t_n) = \frac{1}{\Gamma(1-\alpha)} \int_{s=0}^{t_n} (t_n - s)^{-\alpha} \frac{\partial(v - \bar{v})}{\partial s}(x_m, s) ds. \tag{39b}$$

Set

$$\theta_{n,k} = \frac{\alpha}{\Gamma(1-\alpha)} \int_{s=t_k}^{t_{k+1}} (t_n - s)^{-\alpha-1} (v - \bar{v})(x_m, s) ds \tag{40a}$$

for $k = 0, 1, \dots, n-1$. An integration by parts shows easily that one also has

$$\theta_{n,k} = \frac{1}{\Gamma(1-\alpha)} \int_{s=t_k}^{t_{k+1}} (t_n - s)^{-\alpha} \frac{\partial(v - \bar{v})}{\partial s}(x_m, s) ds \tag{40b}$$

for $k = 0, 1, \dots, n-2$, and then the equivalence of (39a) and (39b) (or a careful integration by parts of (40a)) implies that (40b) is also valid for $k = n-1$. Thus we now have the truncation error formula

$$(D_N^\alpha - D_t^\alpha)u(x_m, t_n) = \sum_{k=0}^{n-1} \theta_{n,k}, \tag{41}$$

where one can use (40a) or (40b) to evaluate each $\theta_{n,k}$.

Denote the temporal piecewise linear interpolant of any suitable function w by

$$w_I(x_m, s) := w(x_m, t_k) + \frac{w(x_m, t_{k+1}) - w(x_m, t_k)}{t_{k+1} - t_k} (s - t_k) \text{ for } s \in I_k := [t_k, t_{k+1}].$$

For $k \geq 1$ and $w \in C^2[t_1, t_n]$, it is well known that

$$\|w - w_I\|_{\infty, I_k} \leq C\tau_{k+1}^2 \|w_{tt}\|_{\infty, I_k} \text{ and } \left\| \frac{\partial(w - w_I)}{\partial t} \right\|_{\infty, I_k} \leq C\tau_{k+1} \|w_{tt}\|_{\infty, I_k}, \quad (42)$$

where

$$\|g\|_{\infty, I_k} := \max_{x \in [0, l], t \in I_k} |g(x, t)|.$$

For $s \in I_k$ with $k \geq 0$, the fitted interpolation error can be written as

$$(v - \bar{v})(x_m, s) = (v - v_I)(x_m, s) + \frac{v(x_m, t_{k+1}) - v(x_m, t_k)}{t_{k+1}^\alpha - t_k^\alpha} [(s^\alpha)_I - s^\alpha]. \quad (43)$$

The bounding of this interpolation error will be split into the two cases of $t_{k+1} \leq 1$ and $t_{k+1} > 1$. In the case where $t_{k+1} \leq 1$, Theorem 1 yields

$$\frac{|v(x_m, t_{k+1}) - v(x_m, t_k)|}{t_{k+1}^\alpha - t_k^\alpha} = \left| \frac{\int_{s=t_k}^{t_{k+1}} \frac{\partial v}{\partial s}(x_m, s) ds}{t_{k+1}^\alpha - t_k^\alpha} \right| \leq C \frac{(t_{k+1}^{2\alpha} - t_k^{2\alpha})}{t_{k+1}^\alpha - t_k^\alpha} \leq C t_{k+1}^\alpha.$$

for $k \geq 0$. Then it follows from (43) that

$$\begin{aligned} |(v - \bar{v})(x_m, s)| &\leq C\tau_{k+1}^2 \|v_{tt}\|_{\infty, I_k} + Ct_{k+1}^\alpha \tau_{k+1}^2 \|(s^\alpha)''\|_{\infty, I_k} \\ &\leq C\tau_{k+1}^2 t_k^{2\alpha-2} + C\tau_{k+1}^2 t_{k+1}^\alpha t_k^{\alpha-2} \\ &\leq C\tau_{k+1}^2 t_k^{2\alpha-2}. \end{aligned}$$

In the other case of $t_{k+1} > 1$, Theorem 3 gives

$$\frac{|v(x_m, t_{k+1}) - v(x_m, t_k)|}{t_{k+1}^\alpha - t_k^\alpha} \leq C \frac{t_{k+1} - t_k}{t_{k+1}^\alpha - t_k^\alpha} \leq Ct_{k+1}^{1-\alpha} \text{ for } k \geq 0.$$

Then (43) yields

$$\begin{aligned} |(v - \bar{v})(x_m, s)| &= |(v - v_I)(x_m, s)| + \left| \frac{v(x_m, t_{k+1}) - v(x_m, t_k)}{t_{k+1}^\alpha - t_k^\alpha} \right| |[(s^\alpha)_I - s^\alpha]| \\ &\leq C\tau_{k+1}^2 \|v_{tt}\|_{\infty, I_k} + Ct_{k+1}^{1-\alpha} \tau_{k+1}^2 \|(s^\alpha)''\|_{\infty, I_k} \\ &\leq C\tau_{k+1}^2 + C\tau_{k+1}^2 t_{k+1}^{1-\alpha} t_{k+1}^{\alpha-2} \\ &\leq C\tau_{k+1}^2. \end{aligned}$$

Combining these two bounds on $v - \bar{v}$ and using an analogous argument to bound the derivative of the interpolation error, we have the interpolation error bounds

$$\|v - \bar{v}\|_{\infty, I_k} \leq C\tau_{k+1}^2 \max\{1, t_k^{2\alpha-2}\} \leq C\tau_{k+1}^2 t_k^{2\alpha-2} \max\{1, t_n^{2-2\alpha}\} \quad (44)$$

and

$$\left\| \frac{\partial(v - \bar{v})}{\partial t} \right\|_{\infty, I_k} \leq C\tau_{k+1} \max\{1, t_k^{2\alpha-2}\}. \quad (45)$$

In the next Lemma these interpolation bounds will be used to bound the $\theta_{n,k}$ in the truncation error (41).

Lemma 2 *There exists a constant C such that for all $n \geq 1$*

$$|(D_N^\alpha - D_t^\alpha)v(x_m, t_n)| \leq C \max\{t_n^\alpha, t_n^{2-\alpha}\} \left[n^{-(2-\alpha)} + n^{-2r\alpha} \right].$$

Proof Fix $n \geq 1$. The argument is based on (41) and (40).

(a) *Bound on $\theta_{n,0}$:* We use (40b). Observe first that, by Theorem 1 and the definition (33) of the basis functions, one has

$$\begin{aligned} \left| \frac{\partial \bar{v}}{\partial t}(x_m, t) \right| &= \left| (v(x_m, t_1) - v(x_m, 0))\phi_0'(t) \right| \\ &= \alpha \frac{t^{\alpha-1}}{t_1^\alpha} \left| \int_{I_1} \frac{\partial v}{\partial s}(x_m, s) ds \right| \\ &\leq Ct^{\alpha-1}t_1^\alpha. \end{aligned}$$

Hence, when $n = 1$, one gets

$$\begin{aligned} |\theta_{1,0}| &\leq \left| \int_{s=0}^{t_1} (t_1 - s)^{-\alpha} \frac{\partial \bar{v}}{\partial s}(x_m, s) ds \right| + \left| \int_{s=0}^{t_1} (t_1 - s)^{-\alpha} \frac{\partial v}{\partial s}(x_m, s) ds \right| \\ &\leq Ct_1^\alpha \int_{s=0}^{t_1} (t_1 - s)^{-\alpha} s^{\alpha-1} ds + \int_{s=0}^{t_1} (t_1 - s)^{-\alpha} s^{2\alpha-1} ds \\ &\leq Ct_1^\alpha, \end{aligned} \quad (46)$$

where we used Theorem 1 and a standard identity [4, Theorem D.6] for the Euler Beta function.

By (41) the proof of the lemma is now complete in the case $n = 1$, so we shall assume that $n > 1$ in the rest of the proof.

Then $(t_n - s)^{-\alpha} \leq (t_n - t_1)^{-\alpha}$ for $s \in I_1$, so for $n > 1$ we have

$$\begin{aligned} |\theta_{n,0}| &\leq \int_{s=0}^{t_1} (t_n - s)^{-\alpha} \left(\left| \frac{\partial \bar{v}}{\partial s}(x_m, s) \right| + \left| \frac{\partial v}{\partial s}(x_m, s) \right| \right) ds \\ &\leq Ct_1^{2\alpha} (t_n - t_1)^{-\alpha} \\ &\leq Ct_1^{2\alpha} t_n^{-\alpha}. \end{aligned} \quad (47)$$

(b) *Bound on $\sum_{k=1}^{\lceil n/2 \rceil - 1} \theta_{n,k}$:* (Here $\lceil \cdot \rceil$ is the usual ceiling function.) Now (40a) gives

$$\begin{aligned}
\left| \sum_{k=1}^{\lceil n/2 \rceil - 1} \theta_{n,k} \right| &\leq \sum_{k=1}^{\lceil n/2 \rceil - 1} \int_{s=t_k}^{t_{k+1}} (t_n - s)^{-\alpha-1} |(v - \bar{v})(x_m, s)| ds \\
&\leq \sum_{k=1}^{\lceil n/2 \rceil - 1} \|v - \bar{v}\|_{\infty, I_k} \int_{s=t_k}^{t_{k+1}} (t_n - t_{\lceil n/2 \rceil})^{-\alpha-1} ds \\
&\leq C \sum_{k=1}^{\lceil n/2 \rceil - 1} \|v - \bar{v}\|_{\infty, I_k} t_n^{-\alpha-1} \tau_{k+1} \\
&\leq C \max\{1, t_n^{2-2\alpha}\} \sum_{k=1}^{\lceil n/2 \rceil - 1} \left(\frac{\tau_{k+1}}{t_k}\right)^3 \left(\frac{t_k}{t_n}\right)^{1+2\alpha} t_n^\alpha, \\
&\leq C \max\{t_n^\alpha, t_n^{2-\alpha}\} \sum_{k=1}^{\lceil n/2 \rceil - 1} k^{-3} (k^r n^{-r})^{(2\alpha+1)} t_k, \\
&= C \max\{t_n^\alpha, t_n^{2-\alpha}\} n^{-r(2\alpha+1)} \sum_{k=1}^{\lceil n/2 \rceil - 1} k^{r(2\alpha+1)-3}, \quad (48)
\end{aligned}$$

where we used the bounds (44) and (32). As in [18, (5.9)], we can use the inequality

$$n^{-r(2\alpha+1)} \sum_{k=1}^{\lceil n/2 \rceil - 1} k^{r(2\alpha+1)-3} \leq C \begin{cases} n^{-r(2\alpha+1)} & \text{if } r(2\alpha+1) < 2, \\ n^{-2} \ln n & \text{if } r(2\alpha+1) = 2, \\ n^{-2} & \text{if } r(2\alpha+1) > 2, \end{cases} \quad (49)$$

to bound the sum in (48).

(c) *Bound on $\sum_{k=\lceil n/2 \rceil}^{n-2} \theta_{n,k}$:* Invoke (40a) and (44), and observe that $\tau_k \leq \tau_n$ and $t_n \geq t_k \geq 2^{-r} t_n$ for $\lceil n/2 \rceil \leq k \leq n$, to get

$$\begin{aligned}
\left| \sum_{k=\lceil n/2 \rceil}^{n-2} \theta_{n,k} \right| &\leq C \left| \int_{s=t_{\lceil n/2 \rceil}}^{t_{n-1}} (t_n - s)^{-\alpha-1} (v - \bar{v})(x_m, s) ds \right| \\
&\leq C \max\{1, t_n^{2-2\alpha}\} \tau_n^2 t_n^{2\alpha-2} \int_{s=t_{\lceil n/2 \rceil}}^{t_{n-1}} (t_n - s)^{-\alpha-1} ds \\
&\leq C \max\{1, t_n^{2-2\alpha}\} \tau_n^2 t_n^{2\alpha-2} (t_n - t_{n-1})^{-\alpha} \\
&= C \max\{t_n^\alpha, t_n^{2-\alpha}\} \left(\frac{\tau_n}{t_n}\right)^{(2-\alpha)} \\
&\leq C \max\{t_n^\alpha, t_n^{2-\alpha}\} n^{-(2-\alpha)}, \quad (50)
\end{aligned}$$

by (32).

(d) *Bound on $\theta_{n,n-1}$* : By (40b) and (45) we have

$$\begin{aligned} |\theta_{n,n-1}| &\leq \left\| \frac{\partial(v - \bar{v})}{\partial t} \right\|_{\infty, I_{n-1}} \int_{s=t_{n-1}}^{t_n} (t_n - s)^{-\alpha} ds \\ &\leq C \max\{1, t_n^{2-2\alpha}\} \tau_n t_n^{2\alpha-2} (t_n - t_{n-1})^{1-\alpha} \\ &\leq C \max\{t_n^\alpha, t_n^{2-\alpha}\} n^{-(2-\alpha)}, \end{aligned} \quad (51)$$

similarly to (50).

Collecting the bounds (46)-(51) yields (for $n > 1$),

$$\begin{aligned} &|(D_N^\alpha - D_t^\alpha)v(x_m, t_n)| \\ &\leq C t_1^{2\alpha} t_n^{-\alpha} + \max\{t_n^\alpha, t_n^{2-\alpha}\} \left[n^{-r(2\alpha+1)} \sum_{k=1}^{\lceil n/2 \rceil - 1} k^{r(\alpha+1)-3} + n^{-(2-\alpha)} \right] \\ &= C \left(\frac{t_1}{t_n} \right)^{2\alpha} t_n^\alpha + \max\{t_n^\alpha, t_n^{2-\alpha}\} \left[n^{-r(2\alpha+1)} \sum_{k=1}^{\lceil n/2 \rceil - 1} k^{r(\alpha+1)-3} + n^{-(2-\alpha)} \right] \\ &\leq C \max\{t_n^\alpha, t_n^{2-\alpha}\} \left[n^{-(2-\alpha)} + n^{-2r\alpha} \right], \end{aligned}$$

which is the desired result.

Lemma 3 *There exists a constant C such that*

$$|(L_{M,N} - (D_t^\alpha + \mathcal{L}))u(x_m, t_n)| \leq C \begin{cases} (t_n^\alpha n^{-\min\{2-\alpha, 2r\alpha\}} + h^2), & \text{for } t_n \leq 1, \\ (T^{2-\alpha} N^{-\min\{2-\alpha, 2r\alpha\}} + h^2), & \text{for } t_n > 1, \end{cases}$$

Proof When $t_n \leq 1$ the result follows immediately from Lemmas 1-2. In the case where $t_n > 1$, we simply note the following: when $r > (2 - \alpha)/(2\alpha)$, from Lemma 2, one has

$$\begin{aligned} |(D_N^\alpha - D_t^\alpha)v(x_m, t_n)| &\leq C t_n^{2-\alpha} n^{-(2-\alpha)} \\ &= C T^{2-\alpha} N^{-(2-\alpha)} \left(\frac{n}{N} \right)^{(r-1)(2-\alpha)} \\ &\leq C T^{2-\alpha} N^{-(2-\alpha)} \end{aligned}$$

and, when $r \leq (2 - \alpha)/(2\alpha)$, one has

$$\begin{aligned} |(D_N^\alpha - D_t^\alpha)v(x_m, t_n)| &\leq C t_n^{2-\alpha} n^{-2r\alpha} \\ &= C T^{2-\alpha} N^{-2r\alpha} \left(\frac{n}{N} \right)^{(2-\alpha)r-2r\alpha} \leq C T^{2-\alpha} N^{-2r\alpha}. \end{aligned}$$

4.2 Stability and error estimates

This section gives error estimates for the finite difference scheme (36). They are obtained from the truncation error estimate of Lemma 3 and a discrete comparison principle together with some suitable barrier functions.

Lemma 4 *The scheme (36) satisfies a discrete maximum principle, viz., if $f \geq 0$ and $\phi \geq 0$ in (36), then the discrete solution satisfies $u_m^n \geq 0$ for all m and n .*

Proof In the scheme (36), the formulation (34) of the approximation to the Caputo time fractional derivative can be written as

$$D_N^\alpha u_m^n = \sum_{k=0}^n \Theta_{nk} u_m^k,$$

where

$$\begin{aligned} \Theta_{nk} &:= -\frac{\alpha}{\Gamma(1-\alpha)} \int_{s=t_{k-1}}^{t_{k+1}} (t_n - s)^{-\alpha-1} \phi_k(s) ds, \quad 0 < k < n, \\ \Theta_{n0} &:= -\frac{1}{t_n^\alpha \Gamma(1-\alpha)} - \frac{\alpha}{\Gamma(1-\alpha)} \int_{s=0}^{t_1} (t_n - s)^{-\alpha-1} \phi_0(s) ds, \\ \Theta_{nn} &:= -\sum_{k=0}^{n-1} \Theta_{nk}, \end{aligned}$$

and ϕ_k are the basis functions (33). The weights Θ_{nk} satisfy

$$\Theta_{nn} > 0 \quad \text{and} \quad \Theta_{nk} < 0 \quad \text{for} \quad 0 \leq k < n,$$

because of the positivity of the basis functions (33). Recalling also the discretisation of the spatial differential operator \mathcal{L} , we see that the matrix associated with the discrete operator $L_{M,N}$ is irreducibly diagonally dominant with positive diagonal entries and non-positive offdiagonal entries. Hence the system matrix is an M -matrix and the result follows.

The discrete maximum principle of Lemma 4 implies a discrete comparison principle, which can be exploited using discrete barrier functions, as is well known. The next lemma gives a very useful criterion for constructing discrete barrier functions.

Lemma 5 *If a grid function $b(x_m, t_n)$ satisfies*

$$b(x_m, 0) = 0 \quad \text{and} \quad b(x_m, t_i) \leq b(x_m, t_j) \quad \text{if} \quad i \leq j, \quad (52)$$

then

$$D_N^\alpha b(x_m, t_n) \geq \frac{1}{\Gamma(1-\alpha)} \frac{b(x_m, t_n)}{t_n^\alpha}. \quad (53)$$

Proof This result follows from the positivity of the basis functions ϕ_k in the derivation of (34).

The next theorem, which is the main result of the paper, gives error estimates for the fitted scheme (36).

Theorem 4 *The solution u_m^n of the scheme (36) satisfies*

$$|u(x_m, t_n) - u_m^n| \leq C \max\{T^{2\alpha}, T^{2-\alpha}\} N^{-\min\{2-\alpha, 2r\alpha\}} + Ch^2.$$

Proof We consider two cases.

Case (i): Assume $2r\alpha > 2 - \alpha$. From Lemma 3, one has the following estimate for the truncation error

$$\begin{aligned} & |(L_{M,N} - (D_t^\alpha + \mathcal{L}))u(x_m, t_n)| \\ & \leq Ct_n^{\alpha - \frac{2-\alpha}{r}} \left[t_n^{\frac{2-\alpha}{r}} n^{-(2-\alpha)} \right] + CT^{2-\alpha} N^{-(2-\alpha)} + Ch^2 \\ & = C \left[t_n^{\alpha - \frac{2-\alpha}{r}} T^{(2-\alpha)/r} + T^{2-\alpha} \right] N^{-(2-\alpha)} + Ch^2. \end{aligned}$$

Consider the barrier function

$$C \left[b_1(x_m, t_n) + (T^{2-\alpha} N^{-(2-\alpha)} + h^2) \Phi(x_m, t_n) \right],$$

where C is a sufficiently large positive constant. The grid function $b_1 \geq 0$ is defined by

$$b_1(x_m, t_n) := t_n^{2\alpha - \frac{2-\alpha}{r}} T^{\frac{2-\alpha}{r}} N^{-(2-\alpha)},$$

and the grid function Φ is given by

$$\Phi(x_m, t_n) := \frac{x_m(l - x_m)}{pl^2}. \quad (54)$$

Observe that b_1 satisfies (52) and the function Φ satisfies

$$0 \leq \Phi(x_m, t_n) \leq \frac{1}{4p}, \quad L_{M,N} \Phi(x_m, t_n) \geq 2p.$$

Then Lemmas 4 and 5 give

$$\begin{aligned} |u(x_m, t_n) - u_m^n| & \leq C \left[b_1(x_m, t_n) + (T^{2-\alpha} N^{-(2-\alpha)} + h^2) \Phi(x_m, t_n) \right] \\ & \leq Ct_n^{2\alpha - \frac{2-\alpha}{r}} T^{\frac{2-\alpha}{r}} N^{-(2-\alpha)} + C(T^{2-\alpha} N^{-(2-\alpha)} + h^2) \\ & = Ct_n^{2\alpha} \left(\frac{T}{t_n} \right)^{\frac{2-\alpha}{r}} N^{-(2-\alpha)} + C(T^{2-\alpha} N^{-(2-\alpha)} + h^2) \\ & \leq C(T^{2-\alpha} + T^{2\alpha}) N^{-(2-\alpha)} + Ch^2. \end{aligned}$$

Case (ii): Assume $2r\alpha \leq 2 - \alpha$. Then Lemma 3 gives

$$\begin{aligned} |(L_{M,N} - (D_t^\alpha + \mathcal{L}))u(x_m, t_n)| & \leq C(t_n^\alpha n^{-2r\alpha} + T^{2-\alpha} N^{-2r\alpha} + h^2) \\ & \leq C \left[(T^{2\alpha} t_n^{-\alpha} + T^{2-\alpha}) N^{-2r\alpha} + h^2 \right]. \end{aligned}$$

We now use the barrier function

$$C [b_2(x_n, t_m) + (T^{2-\alpha} N^{-2r\alpha} + h^2)\Phi(x_m, t_n)],$$

where C is a sufficiently large positive constant, Φ is given in (54) and b_2 is defined by

$$b_2(x_m, t_n) := T^{2\alpha} N^{-2r\alpha} (1 - e^{-t_n/t_1}).$$

Observe that b_2 also satisfies (52). Furthermore, from Lemma 5 we see that

$$D_N^\alpha b_2(x_m, t_n) \geq \frac{1}{\Gamma(1-\alpha)} \frac{b_2(x_m, t_n)}{t_n^\alpha} \geq CT^{2\alpha} \frac{1 - e^{-1}}{\Gamma(1-\alpha)} t_n^{-\alpha} N^{-2r\alpha}$$

for $n \geq 1$. Lemmas 4 and 5 now yield

$$\begin{aligned} |u(x_m, t_n) - u_m^n| &\leq C [b_2(x_m, t_n) + (T^{2-\alpha} N^{-2r\alpha} + h^2)\Phi(x_m, t_n)] \\ &\leq C(T^{2\alpha} + T^{2-\alpha})N^{-2r\alpha} + Ch^2. \end{aligned}$$

In the next two remarks we discuss the error estimates given in Theorem 4.

Remark 5 (Error estimates for the optimal choice of the grading exponent r) Theorem 4 shows that the scheme (36) converges with order $2r\alpha$ if the grading exponent is chosen such that $r \leq (2-\alpha)/(2\alpha)$ and, otherwise, it converges with order $2-\alpha$.

We propose to take $r = \max\{1, (2-\alpha)/(2\alpha)\}$ as the optimal choice of the grading exponent; then the scheme (36) converges with order $2-\alpha$ for all $0 < \alpha < 1$ and the clustering of too many grid points near $t = 0$ is avoided. Thus if $\alpha \geq 2/3$, then the mesh is uniform and Theorem 4 gives

$$|u(x_m, t_n) - u_m^n| \leq CT^{2\alpha} N^{-(2-\alpha)} + Ch^2.$$

On the other hand, if $\alpha < 2/3$, then the mesh is graded and

$$|u(x_m, t_n) - u_m^n| \leq CT^{2-\alpha} N^{-(2-\alpha)} + Ch^2.$$

These error estimates, besides giving the order of convergence of the finite difference scheme (36), show the dependence on the final time T . We shall illustrate in our numerical experiments that these estimates are sharp (see Tables 4, 5 and 6).

Remark 6 (Error estimates for a suboptimal choice of r) The error estimates for $\alpha < 2/3$ and $1 \leq r < (2-\alpha)/(2\alpha)$ —this includes the approximation on a uniform mesh—are not discussed in the previous remark.

In this case, Theorem 4 shows that the time error discretization is bounded by $CT^{2-\alpha} N^{-2r\alpha}$. We have observed numerically that the order of convergence is $N^{-2r\alpha}$, as expected. But for some values of r (e.g., $r = 1$), we have also observed that the dependence on T is $O(T^{2\alpha})$, not $T^{2-\alpha}$.

Some new error estimates are given in this remark that explain this behaviour. If one considers the barrier function

$$C \left(b_2(x_n, t_m) + h^2\Phi(x_m, t_n) + T^{2\alpha} N^{-2r\alpha} t_n^{2(1-\alpha)} \right)$$

one obtains the error estimates

$$\begin{aligned} |u(x_m, t_n) - u_m^n| &\leq C \left(T^{2\alpha} N^{-2r\alpha} + h^2 + T^{2\alpha} N^{-2r\alpha} t_n^{2(1-\alpha)} \right) \\ &\leq CT^{2\alpha} N^{-2r\alpha} \left(1 + t_n^{2(1-\alpha)} \right) + Ch^2, \end{aligned}$$

and therefore

$$|u(x_m, t_n) - u_m^n| \leq CT^{2\alpha} N^{-2r\alpha} + Ch^2, \quad \text{for } t_n \leq 1.$$

Thus, if the maximum error occurs near $t = 0$ the growth rate is $T^{2\alpha}$ but not $T^{2-\alpha}$. This new error estimate is illustrated in the numerical section in Tables 3, 7 and 8.

5 Numerical results

In this section we first give numerical results for two examples with known and unknown exact solutions that exhibit typical behaviour, i.e., their derivatives behave like (4). The examples are approximated with a standard scheme (which uses the classical L1 approximation for the Caputo time-fractional derivative and central difference approximation for the spatial variable; see for example [18]) and the fitted scheme (36). Our results show that the fitted scheme produces more accurate approximations to the solution of both examples. The theoretical orders of convergence (TOC) from Theorem 4 and [18, Theorem 5.3] are included in the tables for comparison purposes.

The section finishes with an example whose exact solution is a smooth function. For this atypical example we find that on a uniform mesh our fitted method converges as the same rate as the classical L1 approximation.

5.1 Numerical examples

Example 1 Consider the following problem:

$$D_t^\alpha u - \frac{\partial^2 u}{\partial x^2} = f(x, t) \quad \text{for } (x, t) \in (0, \pi) \times (0, 1],$$

with initial condition $u(x, 0) = \sin x$ for $0 < x < \pi$ and boundary conditions $u(0, t) = u(\pi, t) = 0$ for $0 \leq t \leq 1$. The function f is chosen such that the exact solution of the problem is

$$u(x, t) = 0.5 [E_{\alpha, 1}(-t^\alpha) + \cos(\pi t/3)] \sin x,$$

which has a typical weak singularity at $t = 0$ (see [18]).

Since the exact solution of Example 1 is known, we can compute the exact errors in all the numerical approximations. The maximum nodal errors are denoted by

$$E^{M,N} := \max_{(x_m, t_n) \in \bar{Q}} |u(x_m, t_n) - u_m^n|$$

and the corresponding rate of convergence are computed using the usual formula

$$\text{rate}_{M,N} := \log_2 \left(\frac{E^{M,N}}{E^{2M,2N}} \right).$$

In [18, Theorem 5.3] it is established that the standard L1 scheme on a graded mesh satisfies the error estimate

$$\max_{(x_m, t_n) \in \bar{Q}} |u(x_m, t_n) - u_m^n| \leq C \left(h^2 + N^{-\min\{2-\alpha, r\alpha\}} \right) \quad (55)$$

for some constant C . Thus if $r = 1$ (uniform mesh) the L1 scheme converges in time with order α , and if $r \geq (2 - \alpha)/\alpha$ it converges with order $2 - \alpha$. The numerical results computed with this scheme for $r = 1$ and $r = (2 - \alpha)/\alpha$ are given in Tables 1 and 2 and they are in agreement with (55). In the case of a uniform mesh we note the slow rates of convergence for small values of α .

Table 1 Standard L1 scheme: Maximum nodal errors and orders of convergence for Example 1 with a uniform mesh and final time $T = 1$; TOC come from (55)

	TOC	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\alpha = 0.2$	0.2	1.855E-2 0.101	1.729E-2 0.109	1.603E-2 0.118	1.477E-2 0.127	1.353E-2
$\alpha = 0.4$	0.4	1.781E-2 0.327	1.420E-2 0.343	1.120E-2 0.356	8.747E-3 0.367	6.784E-3
$\alpha = 0.6$	0.6	9.117E-3 0.575	6.119E-3 0.584	4.081E-3 0.590	2.711E-3 0.594	1.797E-3
$\alpha = 0.8$	0.8	3.067E-3 0.785	1.781E-3 0.795	1.026E-3 0.798	5.901E-4 0.799	3.391E-4

We next use the fitted scheme (36) to generate approximate solutions of Example 1. In Tables 3 and 4 the maximum nodal errors and the orders of convergence are given with $r = 1$ and $r = \max\{1, (2 - \alpha)/(2\alpha)\}$, respectively. Note that when $r = 1$, Theorem 4 indicates that the order is $\min\{2\alpha, 2 - \alpha\}$ and by Remark 5 the order is $2 - \alpha$ if the optimal grading is used. The computed orders of convergence are in agreement with Theorem 4 and Remark 5. Comparing the numerical results for both schemes, we observe that the fitted scheme is more accurate both on uniform and graded meshes.

We now illustrate the dependence of the errors on the final time T . Consider again Example 1 but with final time $T = 10$ instead of $T = 1$. The maximum nodal errors for the fitted scheme using a graded mesh with $r = \max\{1, (2 - \alpha)/(2\alpha)\}$ are displayed in Table 5; they are clearly greater than in Table 4, so

Table 2 Standard L1 scheme: Maximum nodal errors and orders of convergence for Example 1 for a graded mesh with an optimal grading of $r = (2 - \alpha)/\alpha$ and final time $T = 1$; TOC come from (55)

	TOC	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\alpha = 0.2$	1.8	1.933E-4 1.557	6.570E-5 1.620	2.137E-5 1.661	6.761E-6 1.689	2.097E-6
$\alpha = 0.4$	1.6	3.673E-4 1.541	1.262E-4 1.551	4.308E-5 1.558	1.463E-5 1.564	4.948E-6
$\alpha = 0.6$	1.4	7.097E-4 1.349	2.785E-4 1.363	1.083E-4 1.373	4.181E-5 1.381	1.605E-5
$\alpha = 0.8$	1.2	1.099E-3 1.100	5.127E-4 1.115	2.366E-4 1.130	1.081E-4 1.142	4.899E-5

Table 3 Fitted scheme: Maximum nodal errors and orders of convergence for Example 1 on a uniform mesh and final time $T = 1$; TOC come from Theorem 4

	TOC	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\alpha = 0.2$	0.4	1.971E-3 0.251	1.656E-3 0.251	1.392E-3 0.262	1.161E-3 0.275	9.591E-4
$\alpha = 0.4$	0.8	2.207E-3 0.647	1.410E-3 0.678	8.808E-4 0.705	5.401E-4 0.727	3.263E-4
$\alpha = 0.6$	1.2	9.401E-4 1.092	4.409E-4 1.127	2.019E-4 1.151	9.090E-5 1.155	4.081E-5
$\alpha = 0.8$	1.2	3.435E-4 1.181	1.515E-4 1.184	6.670E-5 1.188	2.927E-5 1.192	1.281E-5

Table 4 Fitted scheme: Maximum nodal errors and orders of convergence for Example 1 on a graded mesh with an optimal grading of $r = \max\{1, (2 - \alpha)/(2\alpha)\}$ and final time $T = 1$; TOC come from Theorem 4

	TOC	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\alpha = 0.2$	1.8	1.451E-4 1.568	4.891E-5 1.626	1.584E-5 1.665	4.996E-6 1.692	1.546E-6
$\alpha = 0.4$	1.6	1.366E-4 1.558	4.639E-5 1.486	1.657E-5 1.494	5.883E-6 1.524	2.045E-6
$\alpha = 0.6$	1.4	4.762E-4 1.277	1.965E-4 1.299	7.986E-5 1.319	3.202E-5 1.335	1.270E-5
$\alpha = 0.8$	1.2	3.435E-4 1.181	1.515E-4 1.184	6.670E-5 1.188	2.927E-5 1.192	1.281E-5

there is some dependence on the final time T . In Table 6 we show the computed “growth rates”

$$\log_{10}(E_{T=10}^{M,N}/E_{T=1}^{M,N}),$$

where $E_{T=1}^{M,N}$ and $E_{T=10}^{M,N}$ are the maximum errors for $T = 1$ and $T = 10$ (they are given in Tables 4 and 5, respectively). These numerical results are in agreement with Remark 5 showing that the dependence on T is approximately $O(T^{2-\alpha})$ if $\alpha < 2/3$ and $O(T^{2\alpha})$ if $\alpha \geq 2/3$.

The numerical results for the fitted scheme using a uniform mesh for $T = 10$ are displayed in Table 7, which are again greater than for $T = 1$ (see Table 3).

Table 5 Fitted scheme: Maximum nodal errors and orders of convergence for Example 1 on a graded mesh with an optimal grading of $r = \max\{1, (2 - \alpha)/(2\alpha)\}$ and final time $T = 10$; TOC come from Theorem 4

	TOC	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\alpha = 0.2$	1.8	8.058E-3 1.578	2.699E-3 1.665	8.511E-4 1.681	2.655E-4 1.705	8.145E-5
$\alpha = 0.4$	1.6	6.509E-3 1.510	2.285E-3 1.536	7.877E-4 1.554	2.683E-4 1.566	9.064E-5
$\alpha = 0.6$	1.4	7.169E-3 1.358	2.797E-3 1.373	1.080E-3 1.384	4.138E-4 1.295	1.687E-4
$\alpha = 0.8$	1.2	1.434E-2 1.170	6.374E-3 1.186	2.802E-3 1.193	1.226E-3 1.196	5.352E-4

Table 6 Fitted scheme: Growth rates for Example 1 on a graded mesh with an optimal grading of $r = \max\{1, (2 - \alpha)/(2\alpha)\}$ and final times $T = 1, 10$

	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\alpha = 0.2$	1.745	1.742	1.730	1.725	1.722
$\alpha = 0.4$	1.678	1.693	1.677	1.659	1.647
$\alpha = 0.6$	1.178	1.153	1.131	1.111	1.123
$\alpha = 0.8$	1.621	1.624	1.623	1.622	1.621

In Table 8 we show the computed growth rates from the maximum errors for $T = 1$ (Table 3) and $T = 10$ (Table 7). These numerical results are in agreement with Remark 5 for $\alpha \geq 2/3$ and Remark 6 for $\alpha < 2/3$, showing that the dependence on T is approximately $O(T^{2\alpha})$ for all the values of α considered in these tables.

Table 7 Fitted scheme: Maximum nodal errors and orders of convergence for Example 1 on a uniform mesh and final time $T = 10$; TOC come from Theorem 4

	TOC	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\alpha = 0.2$	0.4	1.908E-3 -0.313	2.370E-3 0.069	2.259E-3 0.172	2.006E-3 0.213	1.731E-3
$\alpha = 0.4$	0.8	5.182E-3 0.100	4.834E-3 0.416	3.624E-3 0.544	2.485E-3 0.616	1.622E-3
$\alpha = 0.6$	1.2	6.184E-3 0.633	3.987E-3 0.808	2.276E-3 0.968	1.164E-3 1.056	5.594E-4
$\alpha = 0.8$	1.2	1.434E-2 1.170	6.374E-3 1.186	2.802E-3 1.193	1.226E-3 1.196	5.352E-4

Example 2 Consider the test problem

$$D_t^\alpha u - \frac{\partial^2 u}{\partial x^2} + (1+x)u = x(\pi-x)(1+t^4) + t^2$$

Table 8 Fitted scheme: Growth rates for Example 1 on a uniform mesh and final times $T = 1, 10$

	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\alpha = 0.2$	-0.014	0.156	0.210	0.238	0.256
$\alpha = 0.4$	0.371	0.535	0.614	0.663	0.696
$\alpha = 0.6$	0.818	0.956	1.052	1.107	1.137
$\alpha = 0.8$	1.621	1.624	1.623	1.622	1.621

for $(x, t) \in Q := (0, \pi) \times (0, 1]$, with

$$\begin{aligned} u(0, t) = 0, \quad u(\pi, t) = 0, \quad \text{for } t \in (0, 1], \\ u(x, 0) = \sin x, \quad \text{for } x \in [0, \pi]. \end{aligned}$$

The exact solution of Example 2 is unknown and the orders of convergence in the computed solutions are estimated using the two-mesh principle [6]. The maximum nodal two-mesh differences are defined by

$$D^{M,N} := \max_{0 \leq m \leq M} \max_{0 \leq n \leq N} |u_m^n - z_{2m}^{2n}|,$$

where z_m^n , with $0 \leq m \leq 2M$ and $0 \leq n \leq 2N$ is the computed solution by the scheme (36) which uses a uniform in the spatial direction with $2M$ mesh intervals, and a graded mesh

$$t_n = (n/(2N))^r \quad \text{for } 0 \leq n \leq 2N,$$

in the temporal direction. The maximum nodal two-mesh differences are used to compute the estimated rate of convergence in a standard way

$$\log_2 \left(\frac{D^{M,N}}{D^{2M,2N}} \right).$$

The maximum nodal two-mesh differences and their corresponding estimated orders of convergence for Example 2 with the fitted scheme are given in Table 9, where the grading exponent is $r = \max\{1, (2 - \alpha)/(2\alpha)\}$ (see Remark 5). The numerical results are in agreement with the theoretical rates of convergence established in Theorem 4.

Finally, we consider an example where the solution is smooth (i.e., all derivatives needed in the numerical analysis are bounded on the closed domain), since this class of problem has been considered by several researchers (but see [17]). For such problems, our earlier analysis can be modified to show that on a uniform mesh the fitted scheme satisfies the error bound

$$|u(x_m, t_n) - u_m^n| \leq CT^{2-\alpha} N^{-(2-\alpha)} + Ch^2 \quad (56)$$

for all m, n .

Table 9 Fitted scheme: Maximum nodal two-mesh differences and orders of convergence for Example 2 on a graded mesh with an optimal grading of $r = \max\{1, (2-\alpha)/(2\alpha)\}$; TOC come from Theorem 4

	TOC	N=M=64	N=M=128	N=M=256	N=M=512	N=M=1024
$\alpha = 0.2$	1.8	7.411E-4 1.604	2.438E-4 1.653	7.749E-5 1.686	2.408E-5 1.709	7.365E-6
$\alpha = 0.4$	1.6	6.979E-4 1.364	2.712E-4 1.397	1.030E-4 1.433	3.813E-5 1.470	1.376E-5
$\alpha = 0.6$	1.4	2.105E-3 1.079	9.965E-4 1.113	4.606E-4 1.200	2.006E-4 1.237	8.506E-5
$\alpha = 0.8$	1.2	1.866E-3 1.074	8.863E-4 1.128	4.056E-4 1.156	1.820E-4 1.175	8.062E-5

Example 3 Take $p = 1, c(x) = x^2$ and choose the solution of (1) to be

$$u(x, t) = (1 + t^3)(4x(1 - x))^2 + 5t^{3+\alpha}, \quad (x, t) \in [0, 1] \times [0, 1].$$

Then the right-hand side f , the initial condition and the boundary conditions are determined by the statement of (1) and our choices of p, c and u .

Example 3 is solved using our fitted scheme on a uniform mesh. The maximum errors and orders of convergence are given in Table 10, where we have taken $M = 4N$ in order that the error from the temporal discretisation of the fractional term dominates the spatial error. It is clear that the method converges with order $2 - \alpha$, in agreement with (56).

Table 10 Fitted scheme on a uniform mesh: Maximum nodal errors and orders of convergence for an example with smooth solution; TOC come from (56)

	TOC	M=64 N=16	M=128 N=32	M=256 N=64	M=512 N=128	M=1024 N=256
$\alpha = 0.2$	1.8	4.832E-3 1.780	1.407E-3 1.784	4.086E-4 1.787	1.184E-4 1.789	3.425E-5
$\alpha = 0.4$	1.6	1.323E-2 1.571	4.451E-3 1.581	1.488E-3 1.587	4.955E-4 1.590	1.645E-4
$\alpha = 0.6$	1.4	3.429E-2 1.371	1.326E-2 1.383	5.083E-3 1.390	1.940E-3 1.394	7.385E-4
$\alpha = 0.8$	1.2	8.410E-2 1.174	3.726E-2 1.186	1.638E-2 1.192	7.167E-3 1.196	3.129E-3

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References

1. Brunner, H., Han, H., Yin, D.: The maximum principle for time-fractional diffusion equations and its application. *Numer. Funct. Anal. Optim.* **36**(10), 1307–1321 (2015)
2. Brunner, H., Ling, L., Yamamoto, M.: Numerical simulations of 2D fractional subdiffusion problems. *J. Comput. Phys.* **229**(18), 6613–6622 (2010)
3. Courant, R., Hilbert, D.: *Methods of mathematical physics. Vol. I.* Interscience Publishers, Inc., New York, N.Y. (1953)
4. Diethelm, K.: The analysis of fractional differential equations, *Lecture Notes in Mathematics*, vol. 2004. Springer-Verlag, Berlin (2010). An application-oriented exposition using differential operators of Caputo type
5. Eliazar, I.I., Shlesinger, M.F.: Fractional motions. *Phys. Rep.* **527**(2), 101–129 (2013)
6. Farrell, P.A., Hegarty, A.F., Miller, J.J.H., O’Riordan, E., Shishkin, G.I.: Robust computational techniques for boundary layers, *Applied Mathematics (Boca Raton)*, vol. 16. Chapman & Hall/CRC, Boca Raton, FL (2000)
7. Gorenflo, R., Kilbas, A.A., Mainardi, F., Rogosin, S.V.: Mittag-Leffler functions, related topics and applications. Springer Monographs in Mathematics. Springer, Heidelberg (2014)
8. Henry, D.: Geometric theory of semilinear parabolic equations, *Lecture Notes in Mathematics*, vol. 840. Springer-Verlag, Berlin-New York (1981)
9. Jin, B., Lazarov, R., Zhou, Z.: Two fully discrete schemes for fractional diffusion and diffusion-wave equations. Arxiv 1404.3800 (2014)
10. Jin, B., Zhou, Z.: An analysis of Galerkin proper orthogonal decomposition for subdiffusion. *ESAIM: M2AN* **51**(1), 89–113 (2017)
11. Luchko, Y.: Initial-boundary-value problems for the one-dimensional time-fractional diffusion equation. *Fract. Calc. Appl. Anal.* **15**(1), 141–160 (2012)
12. Metzler, R., Klafter, J.: The random walk’s guide to anomalous diffusion: a fractional dynamics approach. *Phys. Rep.* **339**(1), 77 (2000)
13. Mustapha, K., Abdallah, B., Furati, K.M.: A discontinuous Petrov-Galerkin method for time-fractional diffusion equations. *SIAM J. Numer. Anal.* **52**(5), 2512–2529 (2014)
14. Mustapha, K., Abdallah, B., Furati, K.M., Nour, M.: A discontinuous Galerkin method for time fractional diffusion equations with variable coefficients. *Numer. Algorithms* **73**(2), 517–534 (2016)
15. Podlubny, I.: Fractional differential equations, *Mathematics in Science and Engineering*, vol. 198. Academic Press Inc., San Diego, CA (1999). An introduction to fractional derivatives, fractional differential equations, to methods of their solution and some of their applications
16. Sakamoto, K., Yamamoto, M.: Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems. *J. Math. Anal. Appl.* **382**(1), 426–447 (2011)
17. Stynes, M.: Too much regularity may force too much uniqueness. *Fract. Calc. Appl. Anal.* **19**(6), 1554–1562 (2016)
18. Stynes, M., O’Riordan, E., Gracia, J.L.: Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation. *SIAM J. Numer. Anal.* **55**(2), 1057–1079 (2017)
19. Vainikko, G.: Inversion of the Riemann-Liouville integral operator and application to Abel equation. *AIP Conference Proceedings* **1648**(1), 150,020 (2015)
20. Vainikko, G.: Which functions are fractionally differentiable? *Z. Anal. Anwend.* **35**(4), 465–487 (2016)