An efficient numerical method for a time-fractional diffusion equation

Zhongdi Cen, Jian Huang, Anbo Le, Aimin Xu
Institute of Mathematics, Zhejiang Wanli University, Ningbo, China

Abstract: A reaction-diffusion problem with a Caputo time derivative is considered. An integral discretization scheme on a graded mesh along with a decomposition of the exact solution is proposed. The truncation error estimate of the discretization scheme is derived by using the remainder formula of the linear interpolation and some inequality estimate techniques. It is proved that the scheme is second-order convergent by applying a difference analogue of Gronwall’s inequality, which exhibits an enhancement in the convergence rate compared with the $L_1$ schemes. Numerical experiments are presented to support the theoretical result.

Keywords: Fractional differential equation; Caputo derivative; singularity; graded mesh

AMS subject classifications: 65M06, 65M12, 65M15

1 Introduction

This article is prompted by recent publications [3, 10, 11] where the authors consider the following initial-boundary value problem

$$D_t^\alpha u(x, t) + Lu(x, t) = f(x, t), \quad (x, t) \in Q := (0, l) \times (0, T], \quad (1.1)$$

$$u(x, 0) = \phi(x), \quad x \in [0, l], \quad (1.2)$$

$$u(0, t) = u(l, t) = 0, \quad t \in (0, T]. \quad (1.3)$$

Here $D_t^\alpha$ denotes a Caputo fractional derivative with $0 < \alpha < 1$,

$$Lu(x, t) := -p \frac{\partial^2 u}{\partial x^2}(x, t) + c(x)u(x, t),$$

$p$ is a positive constant, $c \in C[0, l]$ with $c \geq 0$, $f \in C(Q)$ and $\phi \in C[0, l]$. It is proved in [3, 11] that under reasonable hypotheses on its data, problem (1.1)-(1.3) has a unique solution $u$ which typically exhibits a weak singularity at $t = 0$.

In [10] a finite difference scheme is proposed, which is a combination of the standard $L_1$ approximation for $D_t^\alpha u$ on a graded temporal mesh and the central difference approximation for $Lu$ on a uniform spatial mesh. It is proved that the scheme 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. In [3, 11] a fitted difference scheme and a preprocessed $L_1$ scheme are used to yield an enhanced convergence rate $O(M^{-2} + N^{-\min(2-\alpha, 2r\alpha)})$, respectively.

In the present paper we construct and analyze an integral discretization scheme on a graded mesh along with a decomposition of the exact solution of problem (1.1)-(1.3). The truncation error estimate of the discretization scheme is derived by using the remainder formula of the linear interpolation and some inequality estimate techniques. It is shown that the convergence order...
of our scheme is $O\left(M^{-2} + N^{-2}\right)$ by applying a difference analogue of Gronwall’s inequality, which improves the convergence orders given in [3, 10, 11]. Numerical experiments are provided to validate the theoretical result.

Notation. Throughout the paper, $C$ will denote a generic positive constant that is independent of the mesh. Note that $C$ can take different values in different places. We always use the (pointwise) maximum norm $\|\cdot\|_{\bar{\Omega}}$, where $\bar{\Omega}$ is a closed and bounded set.

2 The continuous problem

As in [3, Lemma 1], it is assumed that $\phi \in C^4[0, l]$, $0 = \phi(0) = \phi''(0) = \phi(l) = \phi''(l) = f(0, t) = f(l, t)$ for $0 \leq t \leq T$, $c \in C^2[0, l]$ and $f, f_x, f_{xx} \in C\left(Q\right)$, and it is shown that the exact solution $u$ of problem (1.1)-(1.3) can be decomposed as

$$u(x, t) = z(x)t^\alpha + \phi(x) + v(x, t), \quad (x, t) \in \bar{Q},$$

where

$$z(x) = \frac{1}{\Gamma(\alpha + 1)} \left(f(x, 0) + p\phi''(x) - c(x)\phi(x)\right),$$

and $v(x, t)$ is the solution of the following initial-boundary value problem

$$(D^\alpha + L)v(x, t) = f(x, t) + g(x, t), \quad (x, t) \in Q, \quad (2.3)$$

$$v(x, 0) = 0, \quad x \in [0, l], \quad (2.4)$$

$$v(0, t) = v(l, t) = 0, \quad t \in (0, T], \quad (2.5)$$

where

$$g(x, t) = -f(x, 0) + pz''(x)t^\alpha - c(x)z(x)t^\alpha.$$

It is proved in [3, Theorem 1], under extra regularity assumptions $f_{tt} (\cdot, t) \in D\left(L^{1/2}\right)$ and $\|f_{tt} (\cdot, t)\|_{L^{1/2}} + t^2 \|f_{ttt} (\cdot, t)\|_{L^{1/2}} \leq C_1$ for all $t \in (0, T]$, where $0 < \rho < 1$ and $C_1$ is a constant independent of $t$, that $v(x, t)$ satisfies

$$\left|\frac{\partial^{k+\ell} v}{\partial x^k \partial t^\ell}\right| \leq C\left(1 + t^{2\alpha - \ell}\right), \quad 0 \leq k + \ell \leq 4, \quad 0 \leq \ell \leq 2$$

for all $(x, t) \in [0, l] \times (0, T]$ and some constant $C$. The similar bounds have been given in [10, Theorem 2.1], but with $2\alpha$ replaced by $\alpha$. From these bounds we know that $v$ is smoother than $u$.

It is shown in [3, Lemma 6.2] that the problem (2.3)-(2.5) can be written as the following equivalent integral-differential equation with a weakly singular kernel

$$v(x, t) = v(x, 0) + \frac{1}{\Gamma(\alpha)} \int_0^t (t - s)^{\alpha - 1} [f(x, s) - L\nu(x, s)] ds + G(x, t), \quad (x, t) \in Q, \quad (2.7)$$

$$v(x, 0) = 0, \quad x \in [0, l], \quad (2.8)$$

$$v(0, t) = v(l, t) = 0, \quad t \in (0, T]. \quad (2.9)$$
Then, we have the following discretization scheme for problem (2.7)-(2.9):

\[
G(x,t) = -\frac{t^\alpha}{(\alpha+1)} f(x,0) + \frac{t^{2\alpha}}{\Gamma(\alpha)} (p z''(x) - c(x) z(x)) B(\alpha + 1, \alpha).
\]

In the following we will discrete this integral-differential equation instead of the differential equation (1.1)-(1.3).

3 Discretization

In this section we describe a numerical scheme for the integral-differential equation (2.7)-(2.9). The numerical scheme is based on a quadrature rule for the integral term and a central difference method for the temporal discretization.

Based on the properties of the exact solution \(v(x,t)\) we construct a graded mesh \(\Omega^{M,N} := \Omega^M \times \Omega^N\), where \(\Omega^M = \{x_i = ih \mid 0 \leq i \leq M, h = i/M\}\) and \(\Omega^N = \{t_j \mid 0 \leq j \leq N, \Delta t_j = t_j - t_{j-1}\}\) with

\[
t_j = \begin{cases} T \left(\frac{t^\alpha}{N}\right)^{2/\alpha}, & j = 1, \\ T \left(\frac{t^\alpha}{N}\right)^{2/\alpha} + T \left(\frac{t^\alpha}{N}\right)^{3/(2\alpha)}, & j = 2, \\ T \left(\frac{t^\alpha}{N}\right)^{2/\alpha} + T \left(\frac{t^\alpha}{N}\right)^{3/(2\alpha)} + T \left[1 - \left(\frac{t^\alpha}{N}\right)^{2/\alpha} - \left(\frac{t^\alpha}{N}\right)^{3/(2\alpha)}\right] \left(\frac{N^2 - 2}{N}\right)^{1/\alpha}, & 3 \leq j \leq N. \end{cases} \tag{3.1}
\]

On this mesh our discrete scheme is second-order convergent. Furthermore, this mesh avoids too many mesh points concentrating around \(t = 0\) compared with the standard graded mesh \(t_j = T \left(\frac{t^\alpha}{N}\right)^{2/\alpha}\) for \(0 \leq j \leq N\) as that in [6][7][9][10], which improves the accuracy.

An approximation to the integral can be obtained by the following quadrature formula

\[
\int_0^t (t_j - s)^{\alpha - 1} \left[ f(x, s) - Lv(x, s) \right] ds 
\approx \sum_{k=1}^j \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha - 1} \left[ \frac{t_k - s}{\Delta t_k} (f(x, t_{k-1}) - Lv(x, t_{k-1})) + \frac{s - t_k}{\Delta t_k} (f(x, t_k) - Lv(x, t_k)) \right] ds.
\]

Then, we have the following discretization scheme for problem (2.7)-(2.9):

\[
\begin{cases}
V^0_i = 0, \\
V^j_i = V^0_i + \frac{1}{\Gamma(\alpha+1)} \sum_{k=1}^j \left\{ \frac{\Delta t_k}{\alpha} (t_j - t_{k-1})^{\alpha+1} - \frac{1}{\alpha+1} (t_j - t_{k-1})^{\alpha} \right\} + \frac{1}{\Gamma(\alpha+1)} \sum_{k=1}^j \left\{ -\Delta t_k (t_j - t_k)^{\alpha} \right\} \\
\quad - \frac{\Delta t_k}{\alpha+1} \left[ (t_j - t_{k-1})^{\alpha+1} - (t_j - t_k)^{\alpha+1} \right] \right\} + \frac{\Delta t_k}{\alpha+1} \left[ (t_j - t_{k-1})^{\alpha+1} - (t_j - t_k)^{\alpha+1} \right] \right\} + \frac{\Delta t_k}{\alpha+1} \left[ (t_j - t_{k-1})^{\alpha+1} - (t_j - t_k)^{\alpha+1} \right] \\
V^0_j = V^j_M = 0,
\end{cases} \tag{3.2}
\]

where \(V^j_i\) is the discrete approximation to the exact solution \(v\) of (2.7)-(2.9) at the mesh point \((x_i, t_j)\) and the discrete operator \(L^M\) is defined as

\[
L^M V^j_i \equiv - p \frac{V^j_{i+1} - 2V^j_i + V^j_{i-1}}{h^2} + c_i V^j_i. \tag{3.3}
\]
4 Convergence analysis

Let \( w^j_i = V^j_i - v(x_i, t_j) \), where \( V^j_i \) is the solution of problem (3.2) and \( v(x_i, t_j) \) is the solution of problem (2.7)-(2.9) at the mesh point \((x_i, t_j)\). Then, the error \( w^j_i \) satisfies the following equation

\[
\begin{align*}
    w^j_i & + \frac{1}{\Gamma(\alpha + 1)} \sum_{k=1}^{j} (t_j - t_{k-1})^{\alpha - 1} \left[ \frac{t_k - s}{\Delta t_k} f(x_i, t_{k-1}) + \frac{s - t_{k-1}}{\Delta t_k} f(x_i, t_k) - f(x_i, s) \right] ds \\
    & + \frac{1}{\Gamma(\alpha + 1)} \sum_{k=1}^{j} (t_j - t_k)^{\alpha} \left[ \frac{t_j - t_{k-1}}{\Delta t_k} (t_j - t_k)^{\alpha + 1} - (t_j - t_k)^{\alpha + 1} \right] L^M w^{k-1}_i \\
    & = R^j_i, \quad 1 \leq i < M, \ 1 \leq j \leq N, \\
    w^0_i & = 0, \quad 1 \leq i < M, \\
    w^j_M & = 0, \quad 1 \leq j \leq N,
\end{align*}
\]

(4.1)

where

\[
R^j_i = \frac{1}{\Gamma(\alpha)} \sum_{k=1}^{j} \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha - 1} \left[ \frac{t_k - s}{\Delta t_k} f(x_i, t_{k-1}) + \frac{s - t_{k-1}}{\Delta t_k} f(x_i, t_k) - f(x_i, s) \right] ds
\]

(4.2)

(4.3)

For estimating the truncation error we need the following remainder formula of Newton interpolation.

**Lemma 4.1** (See [4]) Assume that \( s_0, s_1, \ldots, s_k \in [a, b] \) are distinct. If \( u^{(k)}(s) \) is continuous on \([a, b]\), then

\[
    u [s_0, s_1, \ldots, s_k] = \int_0^1 dy_1 \int_0^{y_1} dy_2 \cdots \int_0^{y_{k-1}} u^{(k)} \left( (1 - y_1)s_0 + (y_1 - y_2)s_1 + \cdots + (y_{k-1} - y_k)s_{k-1} + y_k s_k \right) dy_k.
\]

Next we give the following technical results under the graded mesh \( \Omega^N \).

**Lemma 4.2** Under some regularity conditions on the data, there exists a positive constant \( C \) independent of \( N \) such that

\[
    \left| \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha - 1} \left[ L v(x, s) - \left( \frac{t_k - s}{\Delta t_k} L v(x, t_{k-1}) + \frac{s - t_{k-1}}{\Delta t_k} L v(x, t_k) \right) \right] ds \right| \leq C N^{-2}
\]

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for \( k = 2, 3 \) and \( j \geq k \).

**Proof.** By using the remainder formula of Newton interpolation we have

\[
\left| \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} \left[ L(x, s) - \left( \frac{t_k - s}{\Delta t_k} L(x, t_{k-1}) + \frac{s - t_{k-1}}{\Delta t_k} L(x, t_k) \right) \right] ds \right| \\
\leq \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} |L[x; s, t_{k-1}, t_k](s - t_{k-1})(t_k - s)| ds \\
\leq \int_{t_{k-1}}^{t_k} \int_0^1 \int_0^{y_1} (t_j - s)^{\alpha-1} (s - t_{k-1})(t_k - s) \\
\cdot \left| \frac{\partial^2 L}{\partial t^2}(x, (1-y_1)s + (y_1-y_2)t_{k-1} + y_2 t_k) \right| dy_2 dy_1 ds \\
\leq C \int_{t_{k-1}}^{t_k} \int_0^1 \int_0^{y_1} (t_j - s)^{\alpha-1} (s - t_{k-1})(t_k - s) \\
\cdot \left\{ 1 + \left[ (1-y_1)s + (y_1-y_2)t_{k-1} + y_2 t_k \right]^{2\alpha-2} \right\} dy_2 dy_1 ds \\
(4.5)
\]

for \( k = 2, 3 \), where we have used (2.6). For \( \alpha = \frac{1}{2} \), from (4.5) we have

\[
\left| \int_{t_{k-1}}^{t_k} (t_j - s)^{-1/2} \left[ L(x, s) - \left( \frac{t_k - s}{\Delta t_k} L(x, t_{k-1}) + \frac{s - t_{k-1}}{\Delta t_k} L(x, t_k) \right) \right] ds \right| \\
\leq C (\Delta t_k)^2 \int_{t_{k-1}}^{t_k} (t_j - s)^{-1/2} ds \int_0^1 dy_1 \int_0^{y_1} \left[ (1-y_1)s + (y_1-y_2)t_{k-1} + y_2 t_k \right]^{-1} dy_2 \\
\leq C (\Delta t_k)^2 \int_{t_{k-1}}^{t_k} (t_j - s)^{-1/2} ds \int_0^1 \frac{y_1}{(1-y_1)s + y_1 t_{k-1}} dy_1 \\
\leq C (\Delta t_k)^2 t_{k-1}^{-1} \int_{t_{k-1}}^{t_k} (t_j - s)^{-1/2} ds \\
\leq C (\Delta t_k)^2 t_{k-1}^{-1} \left[ (t_j - t_{k-1})^{1/2} - (t_j - t_k)^{1/2} \right] \\
\leq C N^{-2} \\
(4.6)
\]

with \( k = 2, 3 \). For \( 0 < \alpha < \frac{1}{2} \) and \( \frac{1}{2} < \alpha < 1 \), from (4.5) we have

\[
\left| \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} \left[ L(x, s) - \left( \frac{t_k - s}{\Delta t_k} L(x, t_{k-1}) + \frac{s - t_{k-1}}{\Delta t_k} L(x, t_k) \right) \right] ds \right| \\
\leq \frac{1}{2\alpha - 1} \left\{ [s + (t_k - s)y_1]^{2\alpha-1} - [s - (s - t_{k-1})y_1]^{2\alpha-1} \right\} dy_1 ds \\
\leq C \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} ds \\
\leq C \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} \left[ (t_j - t_{k-1})^{\alpha} - (t_j - t_k)^{\alpha} \right] \\
\leq C N^{-2} \\
(4.7)
\]

with \( k = 2, 3 \), where we have used \( n \leq 2(n - 1) \) for \( n \geq 2 \). Combining (4.6) with (4.7) to complete the proof. □
Lemma 4.3 There exists a positive constant $C$ independent of $N$ such that
\[
\sum_{k=4}^{j} [(t_j - t_{k-1})^\alpha - (t_j - t_k)^\alpha] (\Delta t_k)^2 t_{k-1}^{2\alpha-2} \leq C N^{-2}, \quad 4 \leq j \leq N.
\]

Proof. Let $\lceil s \rceil$ denote the smallest positive integer that is greater than or equal to $s$ for any $s \in \mathbb{R}^+$. Then we have
\[
\sum_{k=4}^{[j/2]} [(t_j - t_{k-1})^\alpha - (t_j - t_k)^\alpha] (\Delta t_k)^2 t_{k-1}^{2\alpha-2} \leq \sum_{k=4}^{[j/2]} \alpha (t_j - t_k)^{\alpha-1} (\Delta t_k)^3 t_{k-1}^{2\alpha-2}
\leq \alpha (t_j - t_{[j/2]})^{\alpha-1} \sum_{k=4}^{[j/2]} (\Delta t_k)^3 t_{k-1}^{2\alpha-2}
\leq C \left( \frac{j-2}{N-2} \right)^{1-1/\alpha} \sum_{k=4}^{[j/2]} \left( \frac{k-2}{N-2} \right)^{1/\alpha} - \left( \frac{k-3}{N-2} \right)^{1/\alpha} \right] \left( \frac{k-3}{N-2} \right)^{2-2/\alpha}
\leq C \left( \frac{j-2}{N-2} \right)^{1-1/\alpha} \left( \frac{1}{N-2} \right)^3 \sum_{k=4}^{[j/2]} \left( \frac{k-2}{N-2} \right)^{3/\alpha-3} \left( \frac{k-3}{N-2} \right)^{2-2/\alpha}
\leq C \left( \frac{1}{N-2} \right)^3 \sum_{k=4}^{[j/2]} \left( \frac{k-2}{N-2} \right)^{1/\alpha-1},
\]
where we have used the mean value theorem and $n \leq 2(n-1)$ for $n \geq 2$. Moreover, we have
\[
\sum_{k=[j/2]+1}^{j} [(t_j - t_{k-1})^\alpha - (t_j - t_k)^\alpha] (\Delta t_k)^2 t_{k-1}^{2\alpha-2} \leq \max_{[j/2]+1 \leq k \leq j} (\Delta t_k)^2 t_{k-1}^{2\alpha-2} \sum_{k=[j/2]+1}^{j} [(t_j - t_{k-1})^\alpha - (t_j - t_k)^\alpha]
\leq t_{[j/2]}^{2\alpha-2} (t_j - t_{[j/2]})^{\alpha} \max_{[j/2]+1 \leq k \leq j} (\Delta t_k)^2
\leq C \left( \frac{[j/2]-2}{N-2} \right)^{2-2/\alpha} \frac{j-2}{N-2} \max_{[j/2]+1 \leq k \leq j} \left[ \left( \frac{k-2}{N-2} \right)^{1/\alpha} - \left( \frac{k-3}{N-2} \right)^{1/\alpha} \right]^2
\leq C \left( \frac{j-2}{N-2} \right)^{2-2/\alpha} \frac{j-2}{N-2} \left( \frac{j-2}{N-2} \right)^{2/\alpha-2} \left( \frac{1}{N-2} \right)^2
\leq C N^{-2},
\]
where we also have used $n \leq 2(n-1)$ for $n \geq 2$. Combining (4.8) with (4.9) to complete the proof. \(\square\)

Now we can give the truncation error estimate of the discretization scheme.
\textbf{Lemma 4.4} Under some regularity conditions on the data, there exists a positive constant \( C \) independently of \( M \) and \( N \) such that the truncation errors of the discretization scheme (3.2) satisfy

\[
|R_i^j| \leq C (M^{-2} + N^{-2}), \quad 1 \leq i \leq M, \ 1 \leq j \leq N. \quad (4.10)
\]

\textbf{Proof.} For the analysis of the truncation errors we distinguish two cases.

\textbf{Case I:} \( j = 1 \).

From (4.4) we have

\[
|R_1^1| \leq \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} \left| \frac{t_1 - s}{\Delta t_1} f(x_i, 0) + \frac{s}{\Delta t_1} f(x_i, t_1) - f(x_i, s) \right| ds
\]

\[
+ \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} |Lv(x_i, s)| ds
\]

\[
+ \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} \left[ \frac{t_1 - s}{\Delta t_1} |Lv(x_i, 0)| + \frac{s}{\Delta t_1} |Lv(x_i, t_1)| \right] ds
\]

\[
+ \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} \frac{t_1 - s}{\Delta t_1} |Lv(x_i, 0) - L^M v(x_i, 0)| ds
\]

\[
+ \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} \frac{s}{\Delta t_1} |Lv(x_i, t_1) - L^M v(x_i, t_1)| ds
\]

\[
\leq C (t_1 + t_1 M^{-2}) \leq CN^{-2}, \quad (4.11)
\]

where we have used the assumptions for \( f \), (2.6), (3.1) and a Taylor expansion for \( v(x, \cdot) \) about \( x_i \). From this we conclude that the lemma holds true for Case I.

\textbf{Case II:} \( 1 < j \leq N \).

We decompose the truncation error into two components as follows

\[
R_i^j = R_i^{j,1} + R_i^{j,2}, \quad (4.12)
\]

where

\[
R_i^{j,1} = \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} \left[ \frac{t_1 - s}{\Delta t_1} f(x_i, 0) + \frac{s}{\Delta t_1} f(x_i, t_1) - f(x_i, s) \right] ds
\]

\[
+ \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} Lv(x_i, s) ds
\]

\[
- \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} \left[ \frac{t_1 - s}{\Delta t_1} Lv(x_i, 0) + \frac{s}{\Delta t_1} Lv(x_i, t_1) \right] ds
\]

\[
+ \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} \frac{t_1 - s}{\Delta t_1} [Lv(x_i, 0) - L^M v(x_i, 0)] ds
\]

\[
+ \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_1 - s)^{\alpha-1} \frac{s}{\Delta t_1} [Lv(x_i, t_1) - L^M v(x_i, t_1)] ds, \quad (4.13)
\]
Similarly to Case I, from (4.13) we have

\[
R_{i,j}^{i,2} = \frac{1}{\Gamma(\alpha)} \sum_{k=2}^{j} \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha - 1} \left[ \frac{t_k - s}{\Delta t_k} f(x_i, t_{k-1}) + \frac{s - t_{k-1}}{\Delta t_k} f(x_i, t_k) - f(x_i, s) \right] ds + \\
\frac{1}{\Gamma(\alpha)} \sum_{k=2}^{j} \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha - 1} L v(x_i, s) ds - \\
\frac{1}{\Gamma(\alpha)} \sum_{k=2}^{j} \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha - 1} \frac{t_k - s}{\Delta t_k} \left[ L v(x_i, t_{k-1}) - L M v(x_i, t_{k-1}) \right] ds + \\
\frac{1}{\Gamma(\alpha)} \sum_{k=2}^{j} \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha - 1} \frac{s - t_{k-1}}{\Delta t_k} \left[ L v(x_i, t_k) - L M v(x_i, t_k) \right] ds. \tag{4.14}
\]

Similarly to Case I, from (4.13) we have

\[
\left| R_{i,j}^{i,1} \right| \leq \frac{1}{\Gamma(\alpha)} \int_{0}^{t_1} (t_j - s)^{\alpha - 1} \left| \frac{t_1 - s}{\Delta t_1} f(x_i, 0) + \frac{s}{\Delta t_1} f(x_i, t_1) - f(x_i, s) \right| ds + \\
\frac{1}{\Gamma(\alpha)} \int_{0}^{t_1} (t_j - s)^{\alpha - 1} \left| L v(x_i, s) \right| ds - \\
\frac{1}{\Gamma(\alpha)} \int_{0}^{t_1} (t_j - s)^{\alpha - 1} \frac{t_1 - s}{\Delta t_1} \left| L v(x_i, 0) + L v(x_i, t_1) \right| ds + \\
\frac{1}{\Gamma(\alpha)} \int_{0}^{t_1} (t_j - s)^{\alpha - 1} \frac{t_1 - s}{\Delta t_1} \left| L v(x_i, 0) - L M v(x_i, t_1) \right| ds + \\
\frac{1}{\Gamma(\alpha)} \int_{0}^{t_1} (t_j - s)^{\alpha - 1} \frac{s}{\Delta t_1} \left| L v(x_i, t_1) - L M v(x_i, t_1) \right| ds \leq C \left[ \frac{t_1}{t_j} - (t_j - t_1)^\alpha \right] \left[ (\Delta t_1)^2 + 1 + M^{-2} \right] \leq C t_1 (t_j - t_1)^{\alpha - 1} \leq C t_1^{\alpha} \leq C N^{-2}, \tag{4.15}
\]

where we also have used the assumptions for \( f \), (2.6), (3.1), the remainder formula of the linear
interpolation for \( f(\cdot,t) \) and a Taylor expansion for \( v(x,\cdot) \) about \( x_i \). From (4.14) we have

\[
|R_i^{1/2}| \leq \frac{1}{\Gamma(\alpha)} \sum_{k=2}^{j} \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} \left| \frac{t_k - s}{\Delta t_k} f(x_i, t_{k-1}) + \frac{s - t_{k-1}}{\Delta t_k} f(x_i, t_k) - f(x_i, s) \right| ds \\
+ \frac{1}{\Gamma(\alpha)} \sum_{k=2}^{j} \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} \left| L v(x_i, s) - \frac{t_k - s}{\Delta t_k} L v(x_i, t_{k-1}) - \frac{s - t_{k-1}}{\Delta t_k} L v(x_i, t_k) \right| ds \\
+ \frac{1}{\Gamma(\alpha)} \sum_{k=2}^{j} \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} \frac{t_k - s}{\Delta t_k} \left| L v(x_i, t_{k-1}) - L^M v(x_i, t_{k-1}) \right| ds \\
+ \frac{1}{\Gamma(\alpha)} \sum_{k=2}^{j} \int_{t_{k-1}}^{t_k} \left| L v(x_i, t_{k-1}) - L^M v(x_i, t_{k-1}) \right| ds \\
+ C N^{-2} + C M^{-2} \sum_{k=2}^{j} \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} \right| ds \\
\leq C \sum_{k=2}^{j} \left[ (t_j - t_{k-1})^\alpha - (t_j - t_k)^\alpha \right] \left[ (\Delta t_k)^2 + M^{-2} \right] + C N^{-2} \\
+ \frac{1}{\Gamma(\alpha)} \sum_{k=4}^{j} \left| L \frac{\partial^2 v}{\partial t^2}(x, \eta_k) \right| (\Delta t_k)^2 \int_{t_{k-1}}^{t_k} (t_j - s)^{\alpha-1} \right| ds \\
\leq C (M^{-2} + N^{-2}) (t_j - t_1)^\alpha + C N^{-2} + C \sum_{k=4}^{j} \left[ (t_j - t_{k-1})^\alpha - (t_j - t_k)^\alpha \right] (\Delta t_k)^2 \int_{t_{k-1}}^{t_k} \right| ds \\
\leq C (M^{-2} + N^{-2}) ,
\]

where we have used the remainder formula of the linear interpolation for \( v(\cdot,t) \) and \( f(\cdot,t) \) with \( \xi_k, \eta_k \in (t_{k-1}, t_k) \), the bounds on \( v(x,t) \) and its derivatives given by (2.6), the assumptions for \( f(x,t) \), Lemmas 4.2 and 4.3. Therefore, from (4.12), (4.15) and (4.16) we conclude that the lemma also holds true for Case II.

Next we give the error estimates for the discretization scheme.

**Theorem 4.5** Let \( v(x,t) \) be the solution of problem (2.7)-(2.9) and \( V \) be the solution of problem (3.2). Then, under some regularity conditions on the data, we have the following error estimate

\[
\| V - v \|_{\Omega M,N} \leq C (M^{-2} + N^{-2}) ,
\]

where \( C \) is a positive constant independent of \( M \) and \( N \). 

9
Proof. From (4.1) we have
\[
\begin{align*}
\frac{d}{dt} w^j_i &= \left( I + \frac{t_j - t_k-1}{\Gamma(\alpha + 2)} \right)^{-1} R^j_i - \frac{1}{\Gamma(\alpha + 1)} \sum_{k=1}^{j} ((t_j - t_k-1)^\alpha - (t_j - t_k)^\alpha) \\
&- \frac{1}{\Gamma(\alpha + 1)} \sum_{k=1}^{j} \left( \frac{1}{\Gamma(\alpha + 2)} \left[ (t_j - t_k-1)^{\alpha+1} - (t_j - t_k)^{\alpha+1} \right] \right) \\
&- \frac{1}{\Gamma(\alpha + 1)} \sum_{k=1}^{j-1} \left( (t_j - t_k)^\alpha + \frac{1}{\Gamma(\alpha + 1)} \left[ (t_j - t_k-1)^{\alpha+1} - (t_j - t_k)^{\alpha+1} \right] \right) \\
&\cdot \left( I + \frac{t_j - t_k}{\Gamma(\alpha + 2)} \right)^{-1} L^M w^k_i.
\end{align*}
\] (4.18)

It is easy to see that the operator \( I + \frac{t_j - t_k}{\Gamma(\alpha + 2)} L^M \) satisfies a discrete maximum principle, and consequently
\[
\left\| \left( I + \frac{t_j - t_k}{\Gamma(\alpha + 2)} L^M \right)^{-1} \right\|_{\Omega^M} \leq 1, \quad 1 \leq j \leq N.
\] (4.19)

Furthermore, applying the result proved in Palencia [8] we have
\[
\left\| \left( I + \frac{t_j - t_k}{\Gamma(\alpha + 2)} L^M \right)^{-1} L^M \right\|_{\Omega^M} \leq d_j, \quad 1 \leq j \leq N,
\] (4.20)

since \( \left( 1 + \frac{t_j - t_k}{\Gamma(\alpha + 2)} \right)^{-1} \) is a rational A-acceptable function, where \( d_j \) is a positive constant. The analogous problems have been discussed in [1, 5].

Therefore, from (4.18)-(4.20) we can obtain
\[
\left\| w^j \right\|_{\Omega^M} \leq z_j + d_j \sum_{k=1}^{j-1} q_k \left\| w^k \right\|_{\Omega^M},
\] (4.21)

where
\[
\begin{align*}
z_k &= \left\| R^k \right\|_{\Omega^M}, \\
q_k &= \frac{1}{\Gamma(\alpha + 2)} \left\{ \frac{1}{\Delta t_k} \left[ (t_j - t_k-1)^{\alpha+1} - (t_j - t_k)^{\alpha+1} \right] \\
&- \frac{1}{\Delta t_{k+1}} \left[ (t_j - t_{k+1})^{\alpha+1} - (t_j - t_{k+1})^{\alpha+1} \right] \right\}, \quad 1 \leq k \leq j.
\end{align*}
\]

Then applying the discrete analogue of Gronwall’s inequality [13, Theorem 3], we have
\[
\left\| w^j \right\|_{\Omega^M} \leq z_j + d_j \prod_{m=1}^{j-1} (1 + d_m q_m) \cdot \sum_{k=1}^{j-1} z_k q_k \prod_{m=1}^{k} (1 + d_m q_m)^{-1}
\] (4.22)

for \( 1 \leq j \leq N \). Lemma 4.4 implies
\[
0 < z_k \leq C \left( M^{-2} + N^{-2} \right), \quad 1 \leq k \leq j.
\] (4.23)
Furthermore, we have

\[
\sum_{k=1}^{j-1} q_k = \frac{1}{\Gamma(\alpha+2)} \sum_{k=1}^{j-1} \left\{ \frac{1}{\Delta t_k} \left[ (t_j - t_{k-1})^{\alpha+1} - (t_j - t_k)^{\alpha+1} \right] - \frac{1}{\Delta t_{k+1}} \left[ (t_j - t_k)^{\alpha+1} - (t_j - t_{k+1})^{\alpha+1} \right] \right\}
= \frac{1}{\Gamma(\alpha+1)} \sum_{k=1}^{j-1} \left[ (t_j - \mu_k)^\alpha - (t_j - \mu_{k+1})^\alpha \right]
= \frac{1}{\Gamma(\alpha+1)} \left[ (t_j - \mu_1)^\alpha - (t_j - \mu_j)^\alpha \right],
\]

(4.24)

where we have used the mean value theorem with \( \mu_k \in (t_{k-1}, t_k) \). Thus we have

\[
\sum_{k=1}^{j-1} \left[ z_k q_k k \prod_{m=1}^{k} (1 + d_m q_m)^{-1} \right] \leq CN^{-2} \sum_{k=1}^{j-1} q_k
\]
\[= C \left( M^{-2} + N^{-2} \right) \left[ (t_j - \mu_1)^\alpha - (t_j - \mu_j)^\alpha \right]
\leq C \left( M^{-2} + N^{-2} \right),
\]

(4.25)

and

\[
\prod_{m=1}^{j-1} (1 + d_m q_m) \leq \exp \left( \sum_{m=1}^{j-1} d_m q_m \right) \leq \exp (C \left[ (t_j - \mu_1)^\alpha - (t_j - \mu_j)^\alpha \right]) \leq C,
\]

(4.26)

where we have used (4.23)-(4.24) and the inequality \((1 + y) \leq e^y\) for \( y \geq -1 \). Hence, combining (4.25)-(4.26) with (4.22) we can obtain

\[
\|w^j\|_{\Omega M} \leq C \left( M^{-2} + N^{-2} \right), \quad 1 \leq j \leq N.
\]

From this we complete the proof. \( \square \)

Then, our approximation \( U^j_i \) of \( u(x_i, t_j) \) can be obtained from (2.1)

\[
U^j_i = z(x_i) t^\alpha_j + \phi(x_i) + V^j_i, \quad 0 \leq i \leq M, \quad 0 \leq j \leq N.
\]

(4.27)

Therefore, from (4.27) and Theorem 4.5 we have

\[
\|U - u\|_{\Omega M, N} \leq C \left( M^{-2} + N^{-2} \right),
\]

(4.28)

which improves the convergence orders given in [3, 10, 11]. There are two reasons for an enhancement in the convergence rate. The first one is that the fractional differential equation is transformed into an equivalent integral-differential equation which reduces the singularity of the integrand function. The other reason is that the decomposition of the exact solution is used and the remainder term \( v \) is smoother than \( u \).
5 Numerical experiments

In this section we verify experimentally the theoretical results obtained in the preceding section. Error estimates and convergence rates for the discrete scheme are presented for the following example which has been given in [3,11].

**Example** Fractional differential equation with non-homogeneous boundary conditions:

\[ D_\alpha^t u - \frac{\partial^2 u}{\partial x^2} = f(x,t), \quad (x,t) \in (0,\pi) \times (0,1], \]
\[ u(x,0) = \sin x, \quad x \in (0,\pi), \]
\[ u(0,t) = u(1,t) = 0, \quad t \in (0,1]. \]

The function \( f(x,t) \) is chosen such that the exact solution is \( u(x,t) = [E_\alpha (-t^\alpha) + t^3] \sin x \), where \( E_\alpha (\cdot) \) is the classical Mittag-Leffler function. The solution \( u(x,t) \) has a typical weak singularity at \( t = 0 \) (see [3,11]).

The maximum error is denoted by

\[ e_{M,N} = \| U - u \|_{\Omega_{M,N}}, \]

and the corresponding convergence rate is computed by

\[ \text{rate}_{M,N} = \log_2 \left( \frac{e_{M,N}}{e_{2M,2N}} \right) \]

for the discrete scheme (3.2). The error estimates and convergence rates in our computed solutions are listed in Table 1. Table 1 shows that the computed solution converges to the exact solution with second-order accuracy and the numerical results do not depend strongly on the value of \( \alpha \), which supports the convergence estimate of Theorem 4.5.

For comparison we also use the standard \( L1 \) scheme [10] with \( r = (2 - \alpha) / \alpha \) (optimal choice) and the preprocessed \( L1 \) scheme [11] with \( r = (2 - \alpha) / (2\alpha) \) (optimal choice) to compute this example. The numerical results are presented in Table 2. From Tables 1 and 2 we confirm that our method proposed in this paper is more accurate and robust than the \( L1 \) scheme and the preprocessed \( L1 \) scheme.

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References

[1] C. Clavero, J.L. Gracia, J.C. Jorge, High-order numerical methods for one-dimensional parabolic singularly perturbed problems with regular layers, *Numer. Meth. Part. Differ. Equ.*, 21(1) (2005) 149-169.

[2] K. Diethelm, *The analysis of fractional differential equations*, in: Lecture Notes in Mathematics, vol. 2004, Springer, Berlin, 2010.
Table 1: Error estimates $e^{M,N}$ and convergence rates $rate^{M,N}$ of the scheme (3.2) for Example

| $M = N$ | 64      | 128     | 256     | 512     | 1024    |
|---------|---------|---------|---------|---------|---------|
| $\alpha = 0.2$ | 1.0185e-3 | 2.7198e-4 | 7.2032e-5 | 1.8931e-5 | 4.9100e-6 |
|         | 1.905   | 1.917   | 1.928   | 1.947   |         |
| $\alpha = 0.4$ | 4.7052e-4 | 1.1803e-4 | 2.9727e-5 | 7.4922e-6 | 1.8869e-6 |
|         | 1.995   | 1.989   | 1.988   | 1.989   |         |
| $\alpha = 0.6$ | 2.7573e-4 | 6.8004e-5 | 1.6902e-5 | 4.2153e-6 | 1.0530e-6 |
|         | 2.020   | 2.008   | 2.003   | 2.001   |         |
| $\alpha = 0.8$ | 1.8272e-4 | 4.4962e-5 | 1.1153e-5 | 2.7776e-6 | 6.9309e-7 |
|         | 2.023   | 2.011   | 2.006   | 2.003   |         |

Table 2: Error estimates $e^{M,N}$ and convergence rates $rate^{M,N}$ of the standard $L1$ scheme ($L1$) \cite{10} and the preprocessed $L1$ scheme (PL1) \cite{11} with optimal $r$ for Example

| $M = N$ | 64      | 128     | 256     | 512     | 1024    |
|---------|---------|---------|---------|---------|---------|
| $\alpha = 0.2$ | L1 4.5112e-3 | 1.3940e-3 | 3.6266e-4 | 2.3831e-4 | 2.6706e-4 |
|         | 1.694   | 1.943   | 0.606   | -0.164  |         |
|         | PL1 1.6443e-3 | 5.2018e-4 | 1.6109e-4 | 4.9137e-5 | 1.4823e-5 |
|         | 1.660   | 1.691   | 1.713   | 1.729   |         |
| $\alpha = 0.4$ | L1 4.6180e-3 | 1.6175e-3 | 5.5659e-4 | 1.8926e-4 | 6.3823e-5 |
|         | 1.514   | 1.539   | 1.556   | 1.568   |         |
|         | PL1 1.6527e-3 | 5.5897e-4 | 1.8773e-4 | 6.2742e-5 | 2.0897e-5 |
|         | 1.564   | 1.574   | 1.581   | 1.586   |         |
| $\alpha = 0.6$ | L1 6.2359e-3 | 2.4091e-3 | 9.2427e-4 | 3.5303e-4 | 1.3446e-4 |
|         | 1.372   | 1.382   | 1.389   | 1.393   |         |
|         | PL1 2.5219e-3 | 9.5577e-4 | 3.6218e-4 | 1.3723e-4 | 5.1999e-5 |
|         | 1.400   | 1.400   | 1.400   | 1.400   |         |
| $\alpha = 0.8$ | L1 1.0663e-2 | 4.6714e-3 | 2.0426e-3 | 8.9194e-4 | 3.8915e-4 |
|         | 1.191   | 1.193   | 1.195   | 1.197   |         |
|         | PL1 5.9732e-3 | 2.6142e-3 | 1.1449e-3 | 5.0145e-4 | 2.1957e-4 |
|         | 1.192   | 1.191   | 1.191   | 1.191   |         |
[3] J.L. Gracia, E. O’Riordan, and M. Stynes, A fitted scheme for a Caputo initial-boundary value problem, *J. Sci. Comput.*, 76(1) (2018) 583-609.

[4] L.C. Hsu, X.H. Wang, Examples and methods in mathematical analysis, Higher Education Press, 1983, Page 234 (in Chinese).

[5] M.K. Kadalbajoo, L.P. Tripathi, and A. Kumar, A cubic B-spline collocation method for a numerical solution of the generalized Black-Scholes equation, *Math. Comput. Model.*, 55(3-4) (2012) 1483-1505.

[6] M. Kolk, A. Pedas, and E. Tamme, Modified spline collocation for linear fractional differential equations, *J. Comput. Appl. Math.*, 283 (2015) 28-40.

[7] N. Kopteva, M. Stynes, An efficient collocation method for a Caputo two-point boundary value problem, *BIT Numer. Math.*, 55 (2015) 1105-1123.

[8] C. Palencia, A stability result for sectorial operators in Banach spaces, *SIAM J. Numer. Anal.*, 30(5) (1993) 1373-1384.

[9] A. Pedas, E. Tamme, Piecewise polynomial collocation for linear boundary value problems of fractional differential equations, *J. Comput. Appl. Math.*, 236 (2012) 3349-3359.

[10] M. Stynes, E. O’Riordan, and J.L. Gracia, Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation, *SIAM J. Numer. Anal.*, 55(2) (2017) 1057-1079.

[11] M. Stynes, J.L. Gracia, Preprocessing schemes for fractional-derivative problems to improve their convergence rates, *Appl. Math. Lett.*, 74 (2017) 187-192.

[12] M. Stynes, J.L. Gracia, A finite difference method for a two-point boundary value problem with a Caputo fractional derivative, *IMA J. Numer. Anal.*, 35 (2015) 689-721.

[13] D. Willett, J.S.W. Wong, On the discrete analogues of some generalizations of Gronwall’s inequality, *Monatsh. Math.*, 69(4) (1965) 362-367.