Finite difference methods for the time fractional diffusion equation on non-uniform meshes

Ya-nan Zhang\textsuperscript{a,}\textsuperscript{*}, Zhi-zhong Sun\textsuperscript{b}, Hong-lin Liaoc

\textsuperscript{a} School of Mathematical Science, Soochow University, Suzhou 215006, People’s Republic of China
\textsuperscript{b} Department of Mathematics, Southeast University, Nanjing 210096, People’s Republic of China
\textsuperscript{c} Institute of Sciences, PLA University of Science and Technology, Nanjing 211101, People’s Republic of China

\section{1. Introduction}

Fractional differential equations have attracted considerable interest in recent years. They are widely applied in various fields of science and engineering \cite{1,2}. The fractional diffusion equations is one class of these equations, which are used in modeling of anomalous diffusive systems, description of fractional random walk, unification of diffusion and wave propagation phenomenon, etc. \cite{3–9}. Consider the fractional diffusion equation

\begin{equation}
\frac{C_0}{\alpha}D_t^\alpha u(x, t) = \Delta u(x, t) + f(x, t),
\end{equation}

where $\Delta$ is Laplacian, $f$ is a known function and $\frac{C_0}{\alpha}D_t^\alpha$ denotes $\alpha$ order Caputo fractional derivative defined as

\begin{equation}
\frac{C_0}{\alpha}D_t^\alpha u(x, t) = \frac{1}{\Gamma(1 - \alpha)} \int_0^t \frac{\partial u(x, s)}{\partial s} (t - s)^{-\alpha} ds, \quad 0 < \alpha < 1.
\end{equation}
In view of definition, the integral term has weakly singular behavior and the character of history dependence. And it is more difficult to approximate the fractional derivative than the classical derivative. Some fundamental methods of discretized fractional calculus can be found in [10], and earlier numerical results for (partial) integro-differential equations with weakly singular kernels can be found in [11–16] and references therein.

A traditional scheme for approximating the Caputo derivative is

\[
\frac{C^\alpha_t u(x, t_n)}{\Gamma(1-\alpha)} = \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^{n} \frac{u(x, t_k) - u(x, t_{k-1})}{t_k - t_{k-1}} \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha} ds + r^n,
\]

where \(0 = t_0 < t_1 < \cdots < t_n\), and \(r^n\) is the local truncation error. The formula (1.3) is termed as the L1 method [1]. For the uniform mesh, i.e., \(t_k - t_{k-1} = \tau\) for all \(k = 1, 2, \ldots, n\), it was proved that \(r^n = O(\tau^{2-\alpha})\) (see [19] or [28]). The L1 method has been widely used for solving the fractional differential equations with Caputo derivatives (see [17–26]). Utilizing the relation between Caputo derivative and Riemann–Liouville fractional derivative, the L1 method was also applied to time fractional diffusion equation with Riemann–Liouville fractional derivative (see [27–30]). High-order approximations such as compact difference scheme [20, 26, 30, 32] and spectral method [28, 29, 31] were applied to improve the spatial accuracy of fractional diffusion equations; however, it is rather difficult to get a high-order time approximation due to the singularity of fractional derivatives.

From the truncation error estimate of the L1 method on uniform time grid, it is clear that the accuracy is dependent on the fractional order \(\alpha\). It is not so surprising since a weakly singular kernel \((t-s)^{-\alpha}\) is contained in the integral. To improve numerical accuracy of the L1 approximation of fractional derivative, it is very natural to consider non-uniform meshes. In fact, the non-uniform mesh methods have been used for solving integro-differential equations with weakly singular for many years. Brunner [33], Tang [34] studied the numerical solution of weakly singular Volterra integral equations by collocation on graded meshes. Recently, Ma [35] investigated this class of equations by the graded mesh methods. Mustapha [36], Yuste and Quintana-Murillo [37] discussed the implicit finite-difference time-stepping method for the time diffusion equation.

Consider Eq. (1.1) with the boundary and initial value conditions

\[
\begin{align*}
&u(x, t)|_{t=0} = 0, \quad x \in \partial \Omega, \quad 0 < t \leq T, \\
&u(x, 0) = \phi(x), \quad x \in \Omega,
\end{align*}
\]

where \(\phi\) is a known function, \(\Omega\) is a bounded domain in \(\mathbb{R}^d\) \((d = 1, 2, 3)\). We assume that the problem has a unique smooth solution. For bounded function \(u(x, t) \neq 0\), it is easy to see from (1.2) that the integrand \(\frac{u(x, t)}{\Gamma(1-\alpha)(t-s)^{-\alpha}}\) is contained in the integral. To improve approximation, it seems that small time-steps are necessary near the singular point \(s = t\) while larger time-steps can be adopted away from the singular point. A different idea is different from the graded meshes used in [33, 34, 36], in which smaller time-steps are employed near \(t = 0\) to compensate the singular behavior at \(t = 0\) of solution.

The main goal of this work is to construct a more accurate method for approximating the Caputo fractional derivative and apply the method to solve the time fractional diffusion equation. Firstly, the L1 approximation of Caputo derivative on non-uniform grids is investigated in detail. For quasi-uniform meshes, the error of the scheme is \(O(N^{\alpha-2})\), where \(N\) is the number of the grid points. This result is the same as that on uniform mesh. By employing a special non-uniform grid, a second order accuracy numerical integration formula is obtained for any \(\alpha \in (0, 1)\). Next, we apply the novel scheme to time discretization of the fractional diffusion problem and obtain a semi-discrete scheme. It is proved that the semi-discrete scheme is unconditionally stable and convergent in \(L^1\) norm. A fully discrete scheme is also suggested where the fourth-order compact method is considered for spatial discretization. We note that, compared with low-order methods, the fourth-order compact method needs less grid points (and then memory and computational costs) to achieve a specified numerical accuracy. Finally, the difference scheme on non-uniform mesh combining with a moving mesh technique is proposed to improve the temporal accuracy of numerical solution.

The rest of the paper is organized as follows. Rigorous analysis of the L1 approximation of Caputo derivative on any nonuniform meshes is addressed in the next section, where a new second-order scheme is obtained by considering a special non-uniform grid. The semi-discrete method is presented and analyzed in Section 3, while the stability and convergence of a fully discrete method is considered in Section 4. Numerical results and the moving mesh technique are given in Section 5. Some comments are presented in the concluding section.

2. Notations and L1 method on non-uniform meshes

For an integer \(N\), we divide the interval \([0, T]\) into \(N\) subintervals with \(0 = t_0 < t_1 < \cdots < t_N = T\). We denote the time steps as

\[
\tau_n = t_n - t_{n-1}, \quad 1 \leq n \leq N,
\]

and let

\[
\tau_{\text{Max}} = \max_{1 \leq i \leq N} \tau_i, \quad \tau_{\text{Min}} = \min_{1 \leq i \leq N} \tau_i.
\]
For any temporal meshes, we have the following result.

**Lemma 2.1.** For $0 < \alpha < 1$, and $g(t) \in C^2[0, T]$, it holds that

$$
\int_{0}^{t_n} g'(s)(t_n - s)^{-\alpha} \, ds = \frac{n}{\tau_k} \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha} \, ds + R_n, \quad 1 \leq n \leq N, \tag{2.1}
$$

and

$$
|R_n| \leq \left( \frac{\tau_n^2}{2(1-\alpha)} + \frac{\tau_{\text{Max}}^2}{8} \right) \tau_n^{-\alpha} \max_{0 \leq t \leq t_n} |g''(t)|.
$$

**Proof.** We write the integral as

$$
\int_{0}^{t_n} g'(s)(t_n - s)^{-\alpha} \, ds = \int_{0}^{t_{n-1}} g'(s)(t_n - s)^{-\alpha} \, ds + \int_{t_{n-1}}^{t_n} g'(s)(t_n - s)^{-\alpha} \, ds \tag{2.2}
$$

and derive the formula (2.1) by two steps. Firstly, using the formula of integration by parts, we obtain

$$
\int_{0}^{t_{n-1}} g'(s)(t_n - s)^{-\alpha} \, ds
= \left[(t_n - s)^{-\alpha} g(s)\right]_{0}^{t_{n-1}} - \alpha \int_{0}^{t_{n-1}} g(s)(t_n - s)^{-\alpha-1} \, ds
= \tau_n^{-\alpha} g(t_{n-1}) - \tau_n^{-\alpha} g(0) - \alpha \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} g(s)(t_n - s)^{-\alpha-1} \, ds
= \tau_n^{-\alpha} g(t_{n-1}) - \tau_n^{-\alpha} g(0) - \alpha \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{(t_k - s)g(t_{k-1}) + (s - t_{k-1})g(t_k)}{\tau_k} (t_n - s)^{-\alpha-1} \, ds - (R_1)^n, \tag{2.3}
$$

where linear interpolation of $g(s)$ is used, and

$$(R_1)^n = \alpha \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{1}{2} g''(\xi_k)(s - t_k)(s - t_{k-1})(t_n - s)^{-\alpha-1} \, ds, \quad \xi_k \in (t_{k-1}, t_k).$$

Noticing that

$$
\alpha \int_{t_{k-1}}^{t_k} (t_k - s)(t_n - s)^{-\alpha-1} \, ds = -\tau_k(t_n - t_{k-1})^{-\alpha} + \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha} \, ds
$$

and

$$
\alpha \int_{t_{k-1}}^{t_k} (s - t_{k-1})(t_n - s)^{-\alpha-1} \, ds = \tau_k(t_n - t_k)^{-\alpha} - \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha} \, ds,
$$

and substituting the two equalities into (2.3), we have

$$
\int_{0}^{t_{n-1}} g'(s)(t_n - s)^{-\alpha} \, ds
= \tau_n^{-\alpha} g(t_{n-1}) - \tau_n^{-\alpha} g(0) + \sum_{k=1}^{n-1} g(t_{k-1})(t_n - t_{k-1})^{-\alpha} - \sum_{k=1}^{n-1} g(t_k)(t_n - t_k)^{-\alpha}
$$
\[ + \sum_{k=1}^{n-1} \frac{g(t_k) - g(t_{k-1})}{\tau_k} \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha} \, ds = (R_1)^n. \]

It is easy to check that the sum of first four terms of the right hand is equal to zero. Thus we get

\[ \int_0^{t_{n-1}} g'(s)(t_n - s)^{-\alpha} \, ds = \sum_{k=1}^{n-1} \frac{g(t_k) - g(t_{k-1})}{\tau_k} \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha} \, ds = (R_1)^n, \quad (2.4) \]

and

\[ \left| (R_1)^n \right| \leq \frac{\alpha}{8} \max_{0 \leq t \leq t_{n-1}} \left| g''(t) \right| \sum_{k=1}^{n-1} \tau_k^2 \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha-1} \, ds \]

\[ \leq \frac{\alpha \tau^2}{8} \max_{0 \leq t \leq t_{n-1}} \left| g''(t) \right| \int_0^{t_{n-1}} (t_n - s)^{-\alpha-1} \, ds \]

\[ = \frac{\tau_{\text{Max}}^2}{8} \max_{0 \leq t \leq t_{n-1}} \left| g''(t) \right| (t_n^\alpha - t_{n-1}^\alpha) \]

\[ \leq \frac{1}{8} \max_{0 \leq t \leq t_{n-1}} \left| g''(t) \right| \tau_{\text{Max}}^\alpha t_n^\alpha. \quad (2.5) \]

Next, utilizing Taylor expansion, we have

\[ \left| g'(s) - \frac{g(t_n) - g(t_{n-1})}{\tau_n} \right| \leq \frac{\tau_n}{2} \max_{t_{n-1} \leq t \leq t_n} \left| g''(t) \right|, \quad t_{n-1} < s < t_n. \]

Then the error in the interval \([t_{n-1}, t_n]\) satisfies

\[ \left| (R_2)^n \right| = \int_{t_{n-1}}^{t_n} g'(s)(t_n - s)^{-\alpha} \, ds - \frac{g(t_n) - g(t_{n-1})}{\tau_n} \int_{t_{n-1}}^{t_n} (t_n - s)^{-\alpha} \, ds \]

\[ \leq \frac{\tau_n^{2-\alpha}}{2(1-\alpha)} \max_{t_{n-1} \leq t \leq t_n} \left| g''(t) \right|. \]

Combining (2.4), (2.5) and the above inequality, we obtain the claimed estimate. \( \square \)

A sequence of meshes is called quasi-uniform if there exists a finite constant \( \beta \), such that

\[ \tau_{\text{Max}} / \tau_{\text{Min}} \leq \beta. \quad (2.6) \]

In this case, it holds that \( \tau_{\text{Max}} \leq \beta T N^{-1} \). And it is seen that \( R^n \) in Lemma 2.1 is of \( \mathcal{O}(N^{\alpha-2}) \) for any quasi-uniform meshes. When \( \beta = 1 \), it holds that \( \tau_n = TN^{-1} \) for all \( n = 1, 2, \ldots, N \), and the meshes is reduced to the uniform mesh. In this case, Lemma 2.1 revisits the well-known estimation of \( L_1 \) norm such as Lemma 4.1 in [19], Lemma 3.1 in [28]

\[ \frac{\tau_{\text{Max}}^\alpha}{2(2-\alpha)} \left[ A_0 g(t_n) - \sum_{k=1}^{n-1} (A_{n-k-1} - A_{n-k}) g(t_k) - A_{n-1} g(0) \right] + \mathcal{O} \left( \tau^{2-\alpha} \right) \]

where \( \tau = T/N \), and \( A_k = (k+1)^{1-\alpha} - k^{1-\alpha} \).

A sequence of meshes is not quasi-uniform if \( \tau_{\text{Max}} / \tau_{\text{Min}} \to +\infty \) as \( N \to +\infty \). In this article, we are also interested in the non-uniform mesh defined as

\[ \tau_n = (N + 1 - n) \mu, \quad 1 \leq n \leq N, \quad (2.7) \]

where \( \mu = \frac{T}{N+1} \). It is to note that the time steps \( \{\tau_n\}_{n=1}^{N} \) is a monotonically decreasing sequence and \( \tau_1 = \mathcal{O}(N^{-1}) \), \( \tau_N = \mathcal{O}(N^{-2}) \).

Utilizing Lemma 2.1, we obtain that \( R^n = \mathcal{O}(N^{2\alpha-2}) \) for the nonuniform mesh (2.7). It seems that the \( L_1 \) method may lose accuracy. In fact, the estimate of \( (R_1)^n \) in Lemma 2.1 can be improved when the non-uniform mesh (2.7) is considered.
Lemma 2.2. For $0 < \alpha < 1$, and $g(t) \in C^2[0, T]$, it holds for the non-uniform mesh (2.7) that

$\left| \int_0^{t_n} g'(s)(t_n - s)^{-\alpha} ds - \sum_{k=1}^{n} \frac{g(t_k) - g(t_{k-1})}{\tau_k} \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha} ds \right|$

$\leq \left( 1 + \alpha + \frac{2^{1-\alpha}}{1-\alpha} \right) \max_{0 \leq t \leq t_n} |g''(t)| \cdot T^{2-\alpha} \cdot (N+1)^{\alpha-2}, \quad 1 \leq n \leq N - 1,$

(2.8)

and

$\left| \int_0^{t_N} g'(s)(t_N - s)^{-\alpha} ds - \sum_{k=1}^{N} \frac{g(t_k) - g(t_{k-1})}{\tau_k} \int_{t_{k-1}}^{t_k} (t_N - s)^{-\alpha} ds \right|$

$\leq \frac{1 + \alpha}{1-\alpha} 2^{-1-\alpha} \max_{0 \leq t \leq T} |g''(t)| \cdot T^{2-\alpha} N^{-2}.$

(2.9)

**Proof.** From the analysis in Lemma 2.1, the truncation error of the numerical integral in $[0, t_{n-1}]$ satisfies

$\left| (R_1)^n \right| \leq \frac{\alpha}{8} \max_{0 \leq t \leq t_{n-1}} |g''(t)| \sum_{k=1}^{n-1} \tau_k^2 \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha-1} ds$

$\leq \frac{\alpha}{8} \max_{0 \leq t \leq t_{n-1}} |g''(t)| \sum_{k=1}^{n-1} \tau_k^3 (t_n - t_k)^{-\alpha-1}.$

It follows from the definition of the mesh (2.7) that $\mu = \frac{2T}{N(N+1)}$, and

$t_n - t_k = \sum_{l=k+1}^{n} \tau_l = \frac{1}{2} (t_n + t_{k+1})(n-k) = \frac{\mu}{2}(n-k)(2N-n-k+1)$,

$\tau_k = (N-k+1)\mu$.

Thus, we have

$\sum_{k=1}^{n-1} \tau_k^3 (t_n - t_k)^{-\alpha-1}$

$= 2^{1+\alpha} \mu^{2-\alpha} \sum_{k=1}^{n-1} (n-k)^{-\alpha-1} (2N-n-k+1)^{2-\alpha} (N-k+1)^3$

$\leq 2^{1+\alpha} \mu^{2-\alpha} \sum_{k=1}^{n-1} (n-k)^{-\alpha-1} (N-k+1)^{2-\alpha}$

$\leq 2^{1+\alpha} N^{2-\alpha} \mu^{2-\alpha} \sum_{k=1}^{n-1} (n-k)^{-\alpha-1}$

$= 8T^{2-\alpha} (N+1)^{\alpha-2} \sum_{k=1}^{n-1} (n-k)^{-\alpha-1}.$

In addition, it is easy to find that

$\sum_{k=1}^{n-1} (n-k)^{-\alpha-1} \leq 1 + \frac{1}{\alpha},$

and then

$\left| (R_1)^n \right| \leq (1 + \alpha) \max_{0 \leq t \leq t_{n-1}} |g''(t)| T^{2-\alpha} (N+1)^{\alpha-2}.$

(2.10)

On the other hand, the truncation error in $[t_{n-1}, t_n]$ is proved to be $O(\tau_n^{2-\alpha})$. Since that $\tau_n \leq \tau_1$ for all $n \geq 1$, we get
\begin{align*}
|\langle R_2 \rangle^n| & \leq \frac{\tau_n^{2-\alpha}}{2(1-\alpha)} \max_{0 \leq t \leq t_{N-1}} |g''(t)| \\
& \leq \frac{\tau_1^{2-\alpha}}{2(1-\alpha)} \max_{0 \leq t \leq t_{N-1}} |g''(t)| \\
& = \frac{1}{1-\alpha} \max_{0 \leq t \leq t_{N-1}} |g''(t)| T^{2-\alpha} (N+1)^{\alpha-2}. 
\end{align*}

Combining (2.10) and (2.11), we get (2.8).

Now we are to prove the estimate (2.9). The error of the numerical integral in [0, t_{N-1}] satisfies

\begin{align*}
|\langle R_1 \rangle^n| & \leq \frac{\alpha}{8} \max_{0 \leq t \leq t_{N-1}} |g''(t)| \sum_{k=1}^{N-1} t_k^3 (t_N - t_k)^{-\alpha-1}.
\end{align*}

Noticing that \( \tau_k = (N + 1 - k) \mu \), and

\[ t_N - t_k = \sum_{l=k+1}^{N} \tau_l = \frac{1}{2} (\tau_N + \tau_{k+1})(N-k) = \frac{\mu}{2} (N-k)(N-k+1), \]

we obtain

\begin{align*}
\sum_{k=1}^{N-1} t_k^3 (t_N - t_k)^{-\alpha-1} & = 2^{1+\alpha} \mu^{2-\alpha} \sum_{k=1}^{N-1} (N-k)^{-1-\alpha} (N-k+1)^{2-\alpha} \\
& = 2^{1+\alpha} \mu^{2-\alpha} \sum_{k=1}^{N-1} (N-k)^{1-2\alpha} \left( \frac{N-k+1}{N-k} \right)^{2-\alpha} \\
& \leq 8 \mu^{2-\alpha} \sum_{k=1}^{N-1} (N-k)^{1-2\alpha}. \tag{2.12}
\end{align*}

In addition,

\begin{align*}
\mu^{1-\alpha} \sum_{k=1}^{N-1} (N-k)^{1-2\alpha} & = \mu^{1-\alpha} \sum_{k=1}^{N-1} k^{1-2\alpha} \leq \frac{\mu^{1-\alpha}}{2-2\alpha} N^{2-2\alpha} \leq \frac{(2T)^{1-\alpha}}{2-2\alpha}. \tag{2.13}
\end{align*}

Substituting (2.13) into (2.12), we get

\begin{align*}
\sum_{k=1}^{N-1} t_k^3 (t_N - t_k)^{-\alpha-1} & \leq 8 \mu \frac{(2T)^{1-\alpha}}{2-2\alpha} \leq \frac{2^{4-\alpha}}{1-\alpha} T^{2-\alpha} N^{-2}
\end{align*}

and then

\begin{align*}
|\langle R_1 \rangle^n| & \leq \frac{2^{1-\alpha}}{1-\alpha} \max_{0 \leq t \leq t_{N-1}} |g''(t)| T^{2-\alpha} N^{-2}. \tag{2.14}
\end{align*}

In addition, \( \tau_N = \mu \) implies that

\begin{align*}
|\langle R_2 \rangle^n| & \leq \frac{(2T)^{2-\alpha}[N(N+1)]^{\alpha-2}}{2(1-\alpha)} \max_{t_{N-1} \leq t \leq t_N} |g''(t)| \\
& \leq \frac{2^{1-\alpha}}{1-\alpha} \max_{t_{N-1} \leq t \leq t_N} |g''(t)| \cdot T^{2-\alpha} N^{2\alpha-4}. \tag{2.15}
\end{align*}

Combining (2.14) and (2.15), we obtain the wanted estimation (2.9) and complete the proof. \( \square \)

\begin{remark}
The estimate (2.9) implies that the \( L^1 \) method of the Caputo derivative on the non-uniform mesh (2.7) is second order. Given a simple function \( y = t^3 \), it is easy to verify that \( \frac{\Gamma(t)}{\Gamma(t/\alpha)} t^{\alpha} = \frac{\Gamma(t/\alpha)}{\Gamma(t)} t^{\alpha} \). We compute the \( 1/2 \) order derivative of \( t^3 \) on the mesh (2.7) and the uniform mesh. Fig. 1 shows the errors by letting \( N = [20, 40, 80, 160, 320, 640] \). It is clear to see that \( L^1 \) method on the mesh (2.7) generates second order convergence rate, while the method on the uniform mesh get the \( 2 - \alpha \) order accuracy.
\end{remark}
3. A semi-discrete difference scheme

In this section, we derive a semi-discrete difference scheme for the fractional diffusion equation (1.1) with boundary and initial conditions (1.4)–(1.5), and prove the stability and convergence.

3.1. Derivation of the difference scheme

For any temporal meshes on \([0, T]\), denote

\[
\begin{align*}
\alpha^n_k &= \frac{1}{\Gamma(1-\alpha)\tau_k} \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha} \, ds \\
&= \frac{1}{\Gamma(2-\alpha)\tau_k} \left[ (t_n - t_{k-1})^{1-\alpha} - (t_n - t_k)^{1-\alpha} \right], \quad 1 \leq k \leq n, \quad 1 \leq n \leq N. \tag{3.1}
\end{align*}
\]

Lemma 3.1. For any \(n = 1, 2, \ldots, N\), and \(\{\alpha^n_k | 1 \leq k \leq n\}\) defined in (3.1), it holds that

\[
\alpha^n_n > \alpha^n_{n-1} > \cdots > \alpha^n_k > \alpha^n_{k-1} > \cdots > \alpha^n_1 > 0. \tag{3.2}
\]

Proof. Taking notice of that

\[
\frac{1}{\tau_k} \int_{t_{k-1}}^{t_k} (t_n - s)^{-\alpha} \, ds = (t_n - \xi_k)^{-\alpha}, \quad \xi_k \in (t_{k-1}, t_k), \tag{3.3}
\]

and \((t_n - s)^{-\alpha}\) is a monotone increasing function, we get the result immediately. \(\square\)

Consider Eq. (1.1) at the time level \(t_n, n = 1, 2, \ldots, N\). Applying Lemma 2.1, we obtain

\[
\sum_{k=1}^{n} [u(x, t_k) - u(x, t_{k-1})] \alpha^n_k = \Delta u(x, t_n) + f(x, t_n) + (R_t)^n(x), \quad 1 \leq n \leq N, \tag{3.4}
\]

where \((R_t)^n(x)\) is the truncation error.

It follows from the initial and boundary conditions (1.4)–(1.5) that

\[
u(x, t_n)|_{\partial\Omega} = 0, \quad x \in \partial\Omega, \quad 1 \leq n \leq N, \tag{3.5}
\]

\[
u(x, 0) = \phi(x), \quad x \in \bar{\Omega}. \tag{3.6}
\]
Omitting the small term \((R_3)^n(x)\) in (3.4) and replacing the function \(u(x, t_k)\) with its numerical approximation \(u^k(x)\) in (3.4)–(3.6), we get the following difference scheme

\[
\sum_{k=1}^{n} \left[ u^k(x) - u^{k-1}(x) \right] a^n_k = \Delta u^n(x) + f(x, t_n), \quad 1 \leq n \leq N, 
\]

(3.7)

\[ u^n(x)|_{\partial \Omega} = 0, \quad x \in \partial \Omega, \quad 1 \leq n \leq N, \]

(3.8)

\[ u^0(x) = \phi(x), \quad x \in \tilde{\Omega}. \]

(3.9)

### 3.2. Stability and \(H^1\) norm convergence

We introduce the inner product, \(L^2\) norm, \(H^1\) seminorm and \(H^1\) norm

\[ \langle v, w \rangle = \int_{\Omega} vw \, dx, \quad \|v\| = \sqrt{\langle v, v \rangle}, \quad \|\nabla v\| = \sqrt{\langle \nabla v, \nabla v \rangle}, \quad \|v\|_1 = \sqrt{\|v\|^2 + \|\nabla v\|^2}, \]

and the Green's first formula

\[ \langle v, \Delta w \rangle + \langle \nabla v, \nabla w \rangle = \oint_{\partial \Omega} v (\nabla w \cdot \vec{n}) \, dS, \]

where \(\nabla\) denotes gradient operator and \(\vec{n}\) is the outward pointing unit normal of surface element \(dS\).

We prove that difference scheme (3.7)–(3.9) is stable to the initial value \(\phi\) and the inhomogeneous term \(f\).

**Theorem 3.1.** For any temporal meshes, the semi-discrete difference scheme (3.7)–(3.9) is unconditionally stable to \(f\) and \(\phi\), i.e.,

\[ \|\Delta u^n\|^2 \leq \|\nabla \phi\|^2 + \frac{T^\alpha \Gamma(1-\alpha)}{2} \max_{1 \leq k \leq N} \|f(\cdot, t_k)\|^2, \quad 1 \leq n \leq N. \]

**Proof.** Firstly, we write (3.7) as

\[ a^n_k u^n(x) - \Delta u^n(x) = \sum_{k=1}^{n-1} (a^n_{k+1} - a^n_k) u^k(x) + a^n_k u^0(x) + f(x, t_n), \quad 1 \leq n \leq N. \]

Taking the inner product of the above equation with \(-2\Delta u^n(x)\), using the Green’s first formula and noticing that \(u^k(x)|_{\partial \Omega} = 0\), we have

\[
2a^n_k \|\nabla u^n\|^2 + 2\|\Delta u^n\|^2 \\
= 2 \sum_{k=1}^{n-1} (a^n_{k+1} - a^n_k) \|\nabla u^k\|^2 \|\nabla u^n\|^2 + 2a^n_k \|\nabla u^0\|^2 \|\nabla u^n\|^2 - 2 \langle f(\cdot, t_n), \Delta u^n \rangle \\
\leq \sum_{k=1}^{n-1} (a^n_{k+1} - a^n_k) \left( \|\nabla u^k\|^2 + \|\nabla u^n\|^2 \right) + a^n_k \left( \|\nabla u^0\|^2 + \|\nabla u^n\|^2 \right) + \frac{1}{2} \|f(\cdot, t_n)\|^2 + 2 \|\Delta u^n\|^2 \\
= \sum_{k=1}^{n-1} (a^n_{k+1} - a^n_k) \|\nabla u^k\|^2 + a^n_k \|\nabla u^0\|^2 + a^n_k \|\nabla u^n\|^2 + \frac{1}{2} \|f(\cdot, t_n)\|^2 + 2 \|\Delta u^n\|^2,
\]

where we have used that \((a^n_k - a^n_{k-1})\) and \(a^n_k\) are positive (see Lemma 3.1). Then

\[ a^n_k \|\nabla u^n\|^2 \leq \sum_{k=1}^{n-1} (a^n_{k+1} - a^n_k) \|\nabla u^k\|^2 + a^n_k \|\nabla u^0\|^2 + \frac{1}{2} \|f(\cdot, t_n)\|^2, \quad 1 \leq n \leq N. \]

Noticing that \(a^n_k = \frac{1}{\Gamma(1-\alpha)} \frac{1}{t_k} \int_0^{t_k} (t_n - s)^{-\alpha} \, ds > \frac{1}{\Gamma(1-\alpha)} \frac{T^\alpha}{T(1-\alpha)}\), we get

\[ a^n_k \|\nabla u^n\|^2 \leq \sum_{k=1}^{n-1} (a^n_{k+1} - a^n_k) \|\nabla u^k\|^2 + a^n_k \left( \|\nabla u^0\|^2 + \frac{T^\alpha \Gamma(1-\alpha)}{2} \|f(\cdot, t_n)\|^2 \right), \quad 1 \leq n \leq N. \]

Denote
\[ E = \|\nabla u^0\|^2 + \frac{T^\alpha \Gamma(1 - \alpha)}{2} \max_{1 \leq i \leq N} \|f(\cdot, t_i)\|^2, \]

the above inequality reduces to
\[ a^n_n \|\nabla u^n\|^2 \leq \sum_{k=1}^{n-1} (a^n_{k+1} - a^n_k) \|\nabla u^k\|^2 + a^n_1 E, \quad 1 \leq n \leq N. \tag{3.10} \]

We prove by induction that
\[ \|\nabla u^n\|^2 \leq E, \quad 1 \leq n \leq N. \]

Letting \( n = 1 \) in (3.10), we get \( \|\nabla u^1\|^2 \leq E \), which means that the conclusion is valid for \( n = 1 \). Assume that the conclusion is valid for \( n = 1, 2, \ldots, m - 1 \), i.e.
\[ \|\nabla u^n\|^2 \leq E, \quad 1 \leq n \leq m - 1. \]

Then
\[ a^m_m \|\nabla u^m\|^2 \leq \sum_{k=1}^{m-1} (a^m_{k+1} - a^m_k) \|\nabla u^k\|^2 + a^m_1 E \]
\[ \leq \sum_{k=1}^{m-1} (a^m_{k+1} - a^m_k) E + a^m_1 E = a^m_mE. \]

This completes the proof. \( \Box \)

Denoting
\[ e^n(x) = u(x, t_n) - u^n(x), \quad 0 \leq n \leq N, \]
we get the error equation of (3.7)–(3.9)
\[ \sum_{k=1}^{n} [e^k(x) - e^{k-1}(x)] a^n_k = \Delta e^n(x) + (R_1)^n(x), \quad 1 \leq n \leq N, \tag{3.11} \]
\[ e^n(x)|_{\partial \Omega} = 0, \quad x \in \partial \Omega, \quad 1 \leq n \leq N, \tag{3.12} \]
\[ e^0(x) = 0, \quad x \in \Omega. \tag{3.13} \]

Applying Theorem 3.1, we have
\[ \|\nabla e^n\|^2 \leq \frac{T^\alpha \Gamma(1 - \alpha)}{2} \max_{1 \leq k \leq N} \|(R_1)k\|^2, \quad 1 \leq n \leq N. \]

For any quasi-uniform meshes, Lemma 2.1 implies that
\[ \max_{1 \leq k \leq N} \|(R_1)k\| \leq C_R \cdot N^{\alpha - 2}, \quad 1 \leq n \leq N, \]
where \( C_R \) is a positive constant that is dependent on \( T, \alpha \) and the exact solution \( u(x, t) \), but independent of \( N \).

For the non-uniform mesh (2.7), we have proved in Lemma 2.2 that \( R^N = O(N^{-2}) \) and pointed out that the L1 approximation on the mesh is a second order formula of the Caputo derivative. However, to obtain the error estimates of the numerical solutions, we need the uniform error bounds on all time levels. Applying Lemma 2.2, we have
\[ \max_{1 \leq k \leq N} \|(R_1)k\| \leq C_R \cdot (N + 1)^{\alpha - 2}, \quad 1 \leq n \leq N. \]

**Theorem 3.2.** Assume that \( u(x, t) \in C_{x,t}^{2,2} \) is the solution of the fractional diffusion equation (1.1) with the initial and boundary conditions (1.4)–(1.5), and \( \{u^n(x)\}_{n=1}^N \) is the solution of (3.7)–(3.9) on the quasi-uniform mesh (2.6) or non-uniform mesh (2.7), then we have
\[ \|\nabla u(\cdot, t_n) - \nabla u^n(\cdot)\| \leq \sqrt{\frac{T^\alpha \Gamma(1 - \alpha)}{2} C_R N^{\alpha - 2}}, \quad 1 \leq n \leq N. \]

Utilizing Poincaré inequality, Theorem 3.2 implies that the solution of (3.7)–(3.9) is convergent in \( H^1 \) norm as \( N \to +\infty \).
4. A fully discrete difference scheme

In this section, we derive a fully discrete difference scheme, where the fourth order compact difference method is used to approximate the spatial Laplacian. We derive the compact scheme and establish the error estimate for one dimensional (1D) problem, and the method can be easily extended to 2D or 3D problems and the corresponding error estimates are valid.

4.1. Derivation of the fully discrete scheme

Consider Eq. (1.1) in \( \Omega = (0, 1) \). For spatial approximation, let \( h = 1/M \) for a positive integer \( M \), and \( x_i = ih \) (\( 0 \leq i \leq M \)). For any grid function \( v = \{ v_i \mid 0 \leq i \leq M \} \), denote

\[
\delta_x v_{i-1/2} = \frac{1}{h} (v_i - v_{i-1}), \quad \delta_x^2 v_i = \frac{1}{h} (\delta_x v_{i+1/2} - \delta_x v_{i-1/2}),
\]

\[
\mathcal{H}_h v_i = \begin{cases} \frac{1}{12} (v_{i+1} + 10v_i + v_{i-1}), & 1 \leq i \leq M - 1, \\ v_i, & i = 0 \text{ or } M. \end{cases}
\]

It is obvious that

\[
\mathcal{H}_h v_i = \left( 1 + \frac{h^2}{12} \delta_x^2 \right) v_i, \quad 1 \leq i \leq M - 1.
\]

**Lemma 4.1.** (See [39, 40]) Let function \( g(x) \in C^6[\Omega], \) and \( \zeta(s) = 5(1-s)^3 - 3(1-s)^5 \), then

\[
\frac{g''(x_{i+1}) + 10g''(x_i) + g''(x_{i-1})}{12} = \frac{g(x_{i+1}) - 2g(x_i) + g(x_{i-1})}{h^2}
+ \frac{h^4}{360} \int_0^1 [g^{(6)}(x_i - sh) + g^{(6)}(x_i + sh)] \zeta(s) \, ds.
\]

Define the grid functions

\[
U^n_i = u(x_i, t_n), \quad f^n_i = f(x_i, t_n), \quad 0 \leq i \leq M, \quad 0 \leq n \leq N.
\]

It follows from the equality (3.4) that

\[
\sum_{k=1}^n (U^n_i - U^{n-1}_i) a_k^n = \frac{\partial^2 u}{\partial x^2}(x_i, t_n) + f^n_i + (R_x)^n_i(x_i), \quad 1 \leq i \leq M - 1, \quad 1 \leq n \leq N,
\]

and then

\[
\sum_{k=1}^n (\mathcal{H}_h U^n_i - \mathcal{H}_h U^{n-1}_i) a_k^n = \mathcal{H}_h \frac{\partial^2 u}{\partial x^2}(x_i, t_n) + \mathcal{H}_h f^n_i + \mathcal{H}_h (R_x)^n_i(x_i),
\]

\[
1 \leq i \leq M - 1, \quad 1 \leq n \leq N. \tag{4.1}
\]

Applying Lemma 4.1, we have

\[
\mathcal{H}_h \frac{\partial^2 u}{\partial x^2}(x_i, t_n) = \delta_x^2 U^n_i + (R_x)^n_i(x_i), \quad 1 \leq i \leq M - 1, \quad 1 \leq n \leq N, \tag{4.2}
\]

where the local truncation errors

\[
(R_x)^n_i(x_i) = \frac{h^4}{360} \int_0^1 \left[ \frac{\partial^6 u}{\partial x^6}(x_i - sh) + \frac{\partial^6 u}{\partial x^6}(x_i + sh) \right] \zeta(s) \, ds.
\]

Substituting (4.2) into (4.1), we get

\[
\sum_{k=1}^n (\mathcal{H}_h U^n_i - \mathcal{H}_h U^{n-1}_i) a_k^n = \delta_x^2 U^n_i + \mathcal{H}_h f^n_i + R^n_i,
\]

\[
1 \leq i \leq M - 1, \quad 1 \leq n \leq N, \tag{4.3}
\]

where \( R^n_i = \mathcal{H}_h (R_x)^n_i(x_i) + (R_x)^n_i(x_i). \)
Lemma 4.3. This completes the proof.

2 Proof. Utilizing discrete Green formula and noticing that
\[ \| \nabla^2 u^n_i \| \leq C_R (N^{a-2} + h^4), \quad 1 \leq i \leq M - 1, \ 1 \leq n \leq N, \]  
(4.4)
where \( C_R \) is a positive constant independent of \( N \) and \( h \).

Combining the initial and boundary value conditions, omitting the small term \( R_i^n \) and replacing the function \( U_i^n \) with its numerical approximation \( u_i^n \), we get the following difference scheme
\[ \sum_{k=1}^{n} (\mathcal{H}_h u_i^k - \mathcal{H}_h u_i^{k-1}) u_i^n = \delta_x^2 u_i^n + \mathcal{H}_h f_i^n, \quad 1 \leq i \leq M - 1, \ 1 \leq n \leq N, \]  
(4.5)
\[ u_0^n = u_M^n = 0, \quad 1 \leq n \leq N, \]  
(4.6)
\[ u_i^0 = \phi(x_i), \quad 0 \leq i \leq M. \]  
(4.7)

4.2. Stability and convergence

We introduce some notations and lemmas which will be used in the stability and convergence analysis. Let \( \mathcal{V}_h = \{ v \mid v = (v_0, v_1, \ldots, v_M), \ v_0 = v_M = 0 \} \). For any \( v, w \in \mathcal{V}_h \), we introduce the discrete inner product, \( L^2 \) norm, \( H^1 \) semi-norm and \( H^1 \) norm as follows:
\[ \langle v, w \rangle_h = h \sum_{i=1}^{M-1} v_i \cdot w_i, \quad \| v \|_h = \sqrt{\langle v, v \rangle_h}, \]  
\[ \| \delta_x v \|_h = \sqrt{h \sum_{i=1}^{M} (\delta_x v_i)^2}, \quad \| v \|_{1,h} = \sqrt{\| v \|_h^2 + \| \delta_x v \|_h^2}. \]

Notations \( \| \mathcal{H}_h v \|_h, \| \delta_x v \|_h \) are defined similarly.

Lemma 4.2. (See [38].) For any grid function \( v \in \mathcal{V}_h \), it holds that
\[ \| v \|_h \leq \frac{1}{\sqrt{h}} \| \delta_x v \|_h. \]

For any grid functions \( v, w \in \mathcal{V}_h \), we define inner product
\[ \langle v, w \rangle_A = h \sum_{i=1}^{M} \delta_x v_{i-\frac{1}{2}} \cdot \delta_x w_{i-\frac{1}{2}} - \frac{h^2}{12} h \sum_{i=1}^{M-1} \delta_x^2 v_i \cdot \delta_x^2 w_i, \]
and the associated norm
\[ \| v \|_A = \sqrt{\langle v, v \rangle_A}. \]

Using the inverse estimate \( \| \delta_x^2 v \|_h \leq \frac{2}{h} \| \delta_x v \|_h \), we obtain
\[ \frac{2}{3} \| \delta_x v \|_h^2 \leq \| v \|_A^2 \leq \| \delta_x v \|_h^2. \]  
(4.8)

The inequality (4.8) and Lemma 4.2 imply that the norm \( \| \cdot \|_A \) is equivalent to the discrete \( H^1 \) norm.

Lemma 4.3. For any grid function \( v, w \in \mathcal{V}_h \), it holds that
\[ -h \sum_{i=1}^{M-1} (\mathcal{H}_h v_i) \cdot \delta_x^2 w_i = \langle v, w \rangle_A. \]

Proof. Utilizing discrete Green formula and noticing that \( v_0 = v_M = w_0 = w_M = 0 \), we have
\[ -h \sum_{i=1}^{M-1} (\mathcal{H}_h v_i) \cdot \delta_x^2 w_i = -h \sum_{i=1}^{M-1} v_i \cdot \delta_x^2 w_i - \frac{h^2}{12} h \sum_{i=1}^{M-1} \delta_x^2 v_i \cdot \delta_x^2 w_i \]
\[ = h \sum_{i=1}^{M} \delta_x v_{i-\frac{1}{2}} \cdot \delta_x w_{i-\frac{1}{2}} - \frac{h^2}{12} h \sum_{i=1}^{M-1} \delta_x^2 v_i \cdot \delta_x^2 w_i. \]

This completes the proof. □
Theorem 4.1. Suppose \(|u_i^n| 0 \leq i \leq M, 1 \leq n \leq N\) is the solution of the difference scheme (4.5)-(4.7) for any temporal meshes. Then it holds that
\[
\|u^n\|^2_A \leq \|\phi\|^2_A + \frac{T^a}{2} \Gamma(1-\alpha) \frac{\max_{1 \leq i \leq N} \|\mathcal{H}_h f_i^n\|^2_h}{2}, \quad 1 \leq n \leq N.
\]

Proof. It follows from (4.5) that
\[
a_n^u \mathcal{H}_h u^n_1 - \delta_x^2 u^n_1 = \sum^{n-1}_{k=1} (a^n_{k+1} - a^n_k) \mathcal{H}_h u^n_k + a^n_1 \mathcal{H}_h u^n_0 + \mathcal{H}_h f^n.
\]

Multiplying the above equation by \(-2h \delta_x^2 u^n_1\), summing over \(i\) for \(i = 1, 2, \ldots, M - 1\), and applying Lemma 4.3, we have
\[
2a_n^u \|u^n\|^2_A + 2\|\delta_x^2 u^n\|^2_h
\]
\[
= 2 \sum^{n-1}_{k=1} (a^n_{k+1} - a^n_k) \|u^n_k\|^2_A + 2a^n_1 \|u^n_0\|^2_A - 2(\mathcal{H}_h f^n, \delta_x^2 u^n)_h
\]
\[
\leq \sum^{n-1}_{k=1} (a^n_{k+1} - a^n_k) (\|u^n_k\|^2_A + \|u^n_0\|^2_A) + a^n_1 (\|u^n_0\|^2_A + \|u^n_1\|^2_A) + \frac{1}{2} \|\mathcal{H}_h f^n\|^2_h + 2\|\delta_x^2 u^n\|^2_h,
\]
i.e.,
\[
a_n^u \|u^n\|^2_A \leq \sum^{n-1}_{k=1} (a^n_{k+1} - a^n_k) \|u^n_k\|^2_A + a^n_1 \|u^n_0\|^2_A + \frac{1}{2} \|\mathcal{H}_h f^n\|^2_h, \quad 1 \leq n \leq N.
\]
The following process is similar to the proof of Theorem 3.1, and we omit it. \(\square\)

We now consider the convergence of the fully discrete scheme (4.5)-(4.7). Denoting
\[
e^n_i = u(x_i, t_n) - u^n_i, \quad 0 \leq i \leq M, 0 \leq n \leq N,
\]
we obtain the error equations
\[
\sum^n_{k=1} (\mathcal{H}_h e^{k+1}_i - \mathcal{H}_h e^k_i) a^n_k = \delta_x^2 e^n_i + R^n_i, \quad 1 \leq i \leq M - 1, 1 \leq n \leq N, \quad (4.9)
\]
\[
e^n_0 = e^n_M = 0, \quad 1 \leq n \leq N, \quad (4.10)
\]
\[
e^n_i = 0, \quad 0 \leq i \leq M. \quad (4.11)
\]

Applying (4.4) and Theorem 4.1, we obtain the convergence result.

Theorem 4.2. Assume that \(u(x, t) \in C^{\alpha, 2}_{x, t}\) is the solution of the 1D fractional diffusion equation (1.1) with boundary and initial conditions (1.4)-(1.5), and \(|u^n_i| 0 \leq i \leq M, 1 \leq n \leq N\) be the solution of the difference scheme (4.5)-(4.7), where the quasi-uniform time mesh (2.6) or non-uniform mesh (2.7) is used in temporal direction, and uniform grid is used in spatial domain. Then it holds that
\[
\|u(x_i, t_n) - u^n_i\|^2_A \leq \frac{T^a}{2} \Gamma(1-\alpha) \frac{C_k(N^{\alpha-2} + h^4)}{2}, \quad 1 \leq n \leq N.
\]

5. Numerical experiment

In this section, we report on computational experiments. Firstly, we consider the problem with the known exact analytical solution to support error estimates and compare our method with the difference scheme on the uniform time mesh (see [26]). Then a moving local refinement technique is introduced, which can improve the temporal accuracy of numerical solution and need low storage requirement.

We consider the 1D problem with an exact analytical solution:
\[
u(x, t) = \sin(\pi x) t^2
\]
in the domain \((0, 1) \times [0, T]\). It can be checked that the corresponding forcing term and boundary and initial conditions are
Table 1
The maximum norm errors and temporal convergence orders \((T = 1)\).

<table>
<thead>
<tr>
<th>(\alpha)</th>
<th>(N)</th>
<th>(e_I(N, M))</th>
<th>(\text{rate}_I)</th>
<th>(e_{II}(N, M))</th>
<th>(\text{rate}_{II})</th>
<th>(e_{III}(N, M))</th>
<th>(\text{rate}_{III})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/4</td>
<td>10</td>
<td>3.5481e−4</td>
<td>*</td>
<td>2.3822e−4</td>
<td>*</td>
<td>1.8583e−4</td>
<td>*</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>1.1159e−4</td>
<td>1.6688</td>
<td>7.1979e−5</td>
<td>1.7267</td>
<td>4.9737e−5</td>
<td>1.9016</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>3.4703e−5</td>
<td>1.6851</td>
<td>2.1644e−5</td>
<td>1.7336</td>
<td>1.3279e−5</td>
<td>1.9052</td>
</tr>
<tr>
<td></td>
<td>80</td>
<td>1.0700e−5</td>
<td>1.6974</td>
<td>6.4865e−6</td>
<td>1.7384</td>
<td>3.5464e−6</td>
<td>1.9046</td>
</tr>
<tr>
<td>1/2</td>
<td>10</td>
<td>1.3218e−3</td>
<td>*</td>
<td>8.8980e−4</td>
<td>*</td>
<td>6.0682e−4</td>
<td>*</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>4.7736e−4</td>
<td>1.4694</td>
<td>3.1184e−4</td>
<td>1.5112</td>
<td>1.8530e−4</td>
<td>1.7114</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>1.7126e−4</td>
<td>1.4789</td>
<td>1.0946e−4</td>
<td>1.5104</td>
<td>5.8020e−5</td>
<td>1.6753</td>
</tr>
<tr>
<td></td>
<td>80</td>
<td>6.1171e−5</td>
<td>1.4853</td>
<td>3.8456e−5</td>
<td>1.5091</td>
<td>1.8586e−5</td>
<td>1.6424</td>
</tr>
<tr>
<td>3/4</td>
<td>10</td>
<td>3.8471e−3</td>
<td>*</td>
<td>2.7279e−3</td>
<td>*</td>
<td>1.9201e−3</td>
<td>*</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>1.6274e−3</td>
<td>1.2412</td>
<td>1.1364e−3</td>
<td>1.2633</td>
<td>7.3525e−4</td>
<td>1.3849</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>6.8665e−4</td>
<td>1.2449</td>
<td>4.7481e−4</td>
<td>1.2591</td>
<td>2.9084e−4</td>
<td>1.3380</td>
</tr>
<tr>
<td></td>
<td>80</td>
<td>2.8929e−4</td>
<td>1.2471</td>
<td>1.9879e−4</td>
<td>1.2561</td>
<td>1.1757e−4</td>
<td>1.3068</td>
</tr>
</tbody>
</table>

Fig. 2. Error curves of the numerical solutions on uniform, quasi-uniform and non-uniform meshes \((M = 100, N = 10)\).

\[
 \begin{align*}
 f(x, t) &= \sin(\pi x) \left[ \pi^2 t^2 + \frac{2}{\Gamma(3-\alpha)} t^{2-\alpha} \right], \\
 u(0, t) &= u(1, t) = 0, \quad \phi(x) = 0.
\end{align*}
\]

Let \(u_I, u_{II}, u_{III}\) be the solutions of the difference scheme \((4.5)-(4.7)\) on uniform mesh, quasi-uniform mesh \((2.6)\) and non-uniform mesh \((2.7)\), respectively. In the runs, we choose \(\tau_1 = \tau_N\) for the quasi-uniform mesh \((2.6)\) and let \(\{\tau_n\}_{n=1}^N\) be an arithmetic sequence. Denote

\[
 e_I(N, M) = \max_{1 \leq i \leq M} |u(x_i, t_N) - (u_I)_i^N|,
\]

and

\[
 \text{rate}_I = \log_2 \left( \frac{e_I(N/2, M)}{e_I(N, M)} \right).
\]

Similar notations \(e_{II}(N, M), \text{rate}_{II}, e_{III}(N, M), \text{rate}_{III}\) can be defined.

We investigate the temporal errors and convergence orders. In this test, we fix \(M = 100\), a value large enough such that the spatial error is negligible as compared with the temporal error. Table 1 presents the maximum norm errors and the temporal convergence orders for \(\alpha = 1/4, 1/2, 3/4\). It is observed that the solutions are more accurate on the two non-uniform meshes, while the convergence order on the non-uniform mesh \((2.7)\) is better.

Fig. 2 shows the absolute errors of \(u_I, u_{II}\) and \(u_{III}\) versus \(t\) when \(\alpha = 1/2\) and \(x = 1/2\).

Next, we test the spatial errors and convergence orders on the two non-uniform meshes by letting \(M\) vary and fixing \(N\) sufficiently large to avoid contamination of the temporal error. Table 2 gives the results at \(T = 1\). It shows that the method gets fourth-order spatial accuracy.

A new method. It is seen from Fig. 2 that large size time steps \(\tau_1, \tau_2, \ldots\) on non-uniform meshes are used initially and lead to poor accuracy of numerical solutions. In order to improve the temporal accuracy of numerical solution, we introduce a moving refinement technique, and illustrate the method on the non-uniform mesh \((2.7)\). Firstly, we introduce fictitious points \(t_{1k}, t_{2k}, \ldots, t_{Jk}\) in the subinterval \([t_{k-1}, t_k]\), and let \(\sigma_1 = \frac{2\tau_k}{(J_k+1)\tau_{Jk+2}}, t_{1k} = t_{k-1} + (J_k + 1)\sigma_k, t_{Jk} = t_{Jk+2}\). Fig. 3 presents the distribution of fictitious points when \(J_k = J_{k+1} = 2\).
The improved numerical method is presented in the following process and \( u(t_k) \) denotes the numerical solution on the time level \( t_k \).

- **step 1.** For given initial value \( u(t_0) \), compute \( u(t_1) \) by using (3.7)-(3.9) on the grid \( t_0 < t_1^{(1)} < t_2^{(1)} < \cdots < t_j^{(1)} < t_1 \).
- **step 2.** Once \( u(t_j) \) are obtained, compute \( u(t_{n+1}) \) by (3.7)-(3.9) on the grid \( t_0 < t_1 < t_2 < \cdots < t_{n-1} < t_n < t_1^{(n+1)} < t_2^{(n+1)} < \cdots < t_j^{(n+1)} < t_{n+1} \).

It is clear that the local grid refinement is used near \( t_0 \) only when we compute \( u(t_n) \). Once \( u(t_n) \) is obtained, the time mesh on the interval \([0, t_n]\) for computation of \( u(t_{n+1}) \) is the same as that of original mesh (2.7). The main advantage of the method is that it can improve the accuracy of \( u(t_k) \) and then get more accurate solution \( u(t_n) \). In this process, there are only \( J_k \) vectors need to be restored additionally, which is very small compared with the number of grid points on the original mesh.

We now analyze the stability of the improved method. For any temporal meshes, **Theorem 3.1** indicates that the difference scheme (3.7)-(3.9) is unconditionally stable to \( f \) and \( \phi \), i.e.,

\[
\|\nabla u^n\|^2 \leq \|\nabla \phi\|^2 + \frac{T^\alpha \Gamma(1-\alpha)}{2} \max_{1 \leq k \leq n} \left\| f\left(\cdot, t_k\right)\right\|^2, \quad 1 \leq n \leq N. \tag{5.1}
\]

For convenience, we denote a known constant

\[
M = \|\nabla \phi\|^2 + \frac{T^\alpha \Gamma(1-\alpha)}{2} \max_{1 \leq k \leq n} \left\| f\left(\cdot, t_k\right)\right\|^2, \quad \max_{1 \leq j \leq J} \left\| f\left(\cdot, t_j^{(0)}\right)\right\|^2).
\]

When we compute \( u(t_1) \) from **step 1**, it follows from (5.1) that \( \|\nabla u(\cdot,t_1)\|^2 \leq M \). Similarly, when we compute \( u(t_2) \) on a new time grid (**step 2**), (5.1) also implies that \( \|\nabla u(\cdot,t_2)\|^2 \leq M \). Thus the stability can be obtained easily by using induction method because we have found a uniform bound \( M \) for all the numerical solutions.

In order to show the effectiveness, we compute the problem by the improved method, and denote \( u_{IV} \) as the corresponding solutions. The notation \( e_{IV}(N, M) \) is defined similarly. For simplicity, we choose two fictitious points in each subinterval, i.e., \( J_k = 2 \) for all \( 1 \leq k \leq N \). Fig. 4 shows the absolute errors of \( u_1, u_{IV} \) and \( u_{IV} \) when \( \alpha = 1/2 \) and \( \nu = 1/2 \). It is clear to see that the improved method enhance the accuracy successfully.

For the given \( N \) and \( J_k \), one need solve \( \sum_{k=1}^{N}(J_k + 1) \) linear systems to obtain \( u(T) \) by using the improved method. To this end, we choose \( N = [10, 30, 90] \) for the improved method, while let \( N = [30, 90, 270] \) for the L1 method on uniform mesh [26], and compute the temporal error and CPU time. Thus the number of linear systems need to be solved for the two methods are the same. Fortunately, the improved method needs fewer storage and is computational efficient. **Table 3** presents the numerical results and shows the efficiency of the improved method.

Above numerical results are carried out for the fixed time interval. Sometimes, we need to evolve a new time end \( T_2 > T_1 \) after we computed the solution on the interval \([0, T_1]\). In this case, the new time grid points \( t_1, t_2, \ldots \) may be different from the previous ones because the nonuniform meshes are used. If we recompute the solutions at these new grid points, the computational cost will be increased and the method is not efficient. To this end, we present an easy way to avoid recomputation at these grid points. For example, we have computed the solution on the interval \([0, T_1]\) with the time grid

\[ 0 = t_1 < t_2 < \cdots < t_{N_1} = T_1, \]

and we want to evolve the new time end \( T_2 > T_1 \). A natural way is to use the same grid points on the interval \([0, T_1]\), i.e.,

\[ 0 = t_1 < t_2 < \cdots < t_{N_1} = T_1 < t_{N_1+1} < t_{N_1+2} < \cdots < t_{N_1+N_2} = T_2. \]
Table 3
The errors and CPU time (seconds) of the L1 method on uniform mesh [26] and the improved method.

<table>
<thead>
<tr>
<th>α</th>
<th>N</th>
<th>ε₁(N, M)</th>
<th>CPU (s)</th>
<th>N</th>
<th>εIV(N, M)</th>
<th>CPU (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.7</td>
<td>30</td>
<td>7.6086e−4</td>
<td>0.8910</td>
<td>10</td>
<td>6.3482e−4</td>
<td>0.3335</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>1.8334e−4</td>
<td>7.9142</td>
<td>30</td>
<td>1.2807e−4</td>
<td>2.7909</td>
</tr>
<tr>
<td></td>
<td>270</td>
<td>4.4069e−5</td>
<td>71.6312</td>
<td>90</td>
<td>2.7171e−5</td>
<td>24.3402</td>
</tr>
<tr>
<td>0.8</td>
<td>30</td>
<td>1.2649e−3</td>
<td>0.8807</td>
<td>10</td>
<td>8.9663e−4</td>
<td>0.3444</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>3.3929e−4</td>
<td>7.9444</td>
<td>30</td>
<td>2.1762e−4</td>
<td>2.8226</td>
</tr>
<tr>
<td></td>
<td>270</td>
<td>9.0889e−5</td>
<td>72.3050</td>
<td>90</td>
<td>5.4873e−5</td>
<td>24.5395</td>
</tr>
<tr>
<td>0.9</td>
<td>30</td>
<td>2.0778e−3</td>
<td>0.8867</td>
<td>10</td>
<td>1.3392e−3</td>
<td>0.3418</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>6.2114e−4</td>
<td>8.0382</td>
<td>30</td>
<td>3.9020e−4</td>
<td>2.8274</td>
</tr>
<tr>
<td></td>
<td>270</td>
<td>1.8558e−4</td>
<td>72.5664</td>
<td>90</td>
<td>1.1499e−4</td>
<td>24.6306</td>
</tr>
</tbody>
</table>

We can evolve tₙ₊₁ by using the previous points and do not need to recompute these points. Since we have proved that
difference scheme is unconditionally stable on any temporal meshes, the solutions we obtained in the above process are
reliable. If the time grid is quasi-uniform, the error estimate can be obtained directly. In order to improve the computational
efficiency, we can ignore some grid points in the previous time intervals which are far from the current time level, and these
grid points can be seen as the fictitious points in the improved method.

6. Conclusion

In this article, we analyzed the error bounds of the L1 method on non-uniform meshes firstly, and got a second order
formula for computing Caputo derivative on a special non-uniform mesh. Then we applied the method to solve fractional
diffusion equation in a bounded domain Ω ∈ Rᵈ and proved that the corresponding semi-discrete scheme is unconditionally
stable and convergent in H¹ norm. Combining with other numerical methods in spatial direction, one can derive the full-
discrete scheme, for example, the finite difference/spectral method [28]. We derived a compact difference scheme, which
has fourth order spatial accuracy, and established the corresponding error estimate. The method can be easily extended to
high dimensional problem as well as the problem with other boundary conditions. Finally, we presented a moving local re-
finement technique on the non-uniform mesh by introducing fictitious points in each subinterval. The main advantage of the
technique is that it improves the accuracy but does not increase the memory. Numerical comparison shows the efficiency.

In a further work, we plan to investigate the error analysis of the local refinement technique, as well as study the L1
method on other special meshes, such as suitable graded meshes according to the fractional order α.

Acknowledgements

The authors would like to thank the referees for their valuable comments to improve the paper.

References


